

# **WACCM**

## **Introduction and Results**

**D. Kinnison**

**GMI Science Team Meeting**

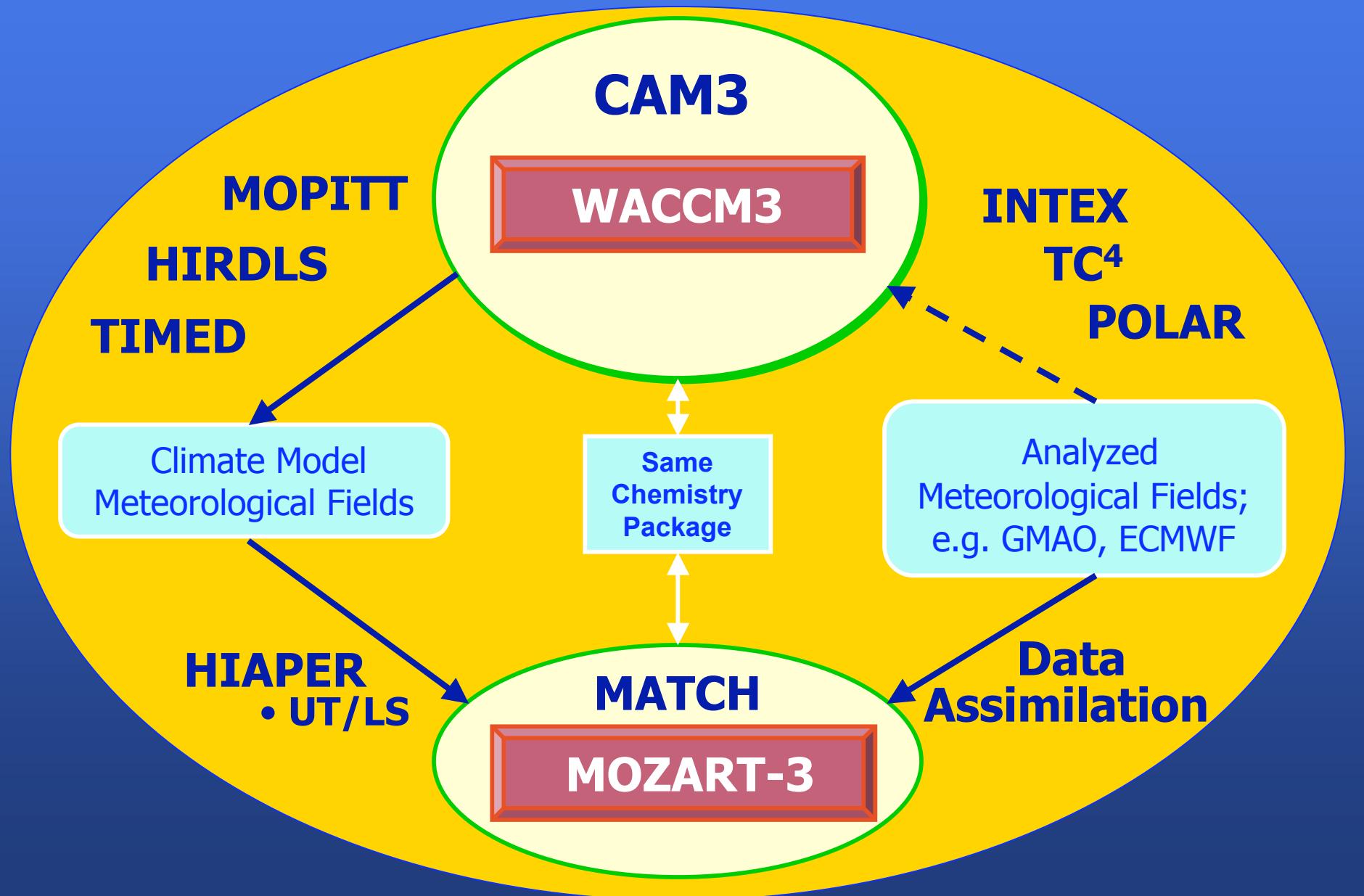
`dkin@ucar.edu`

303-497-1469

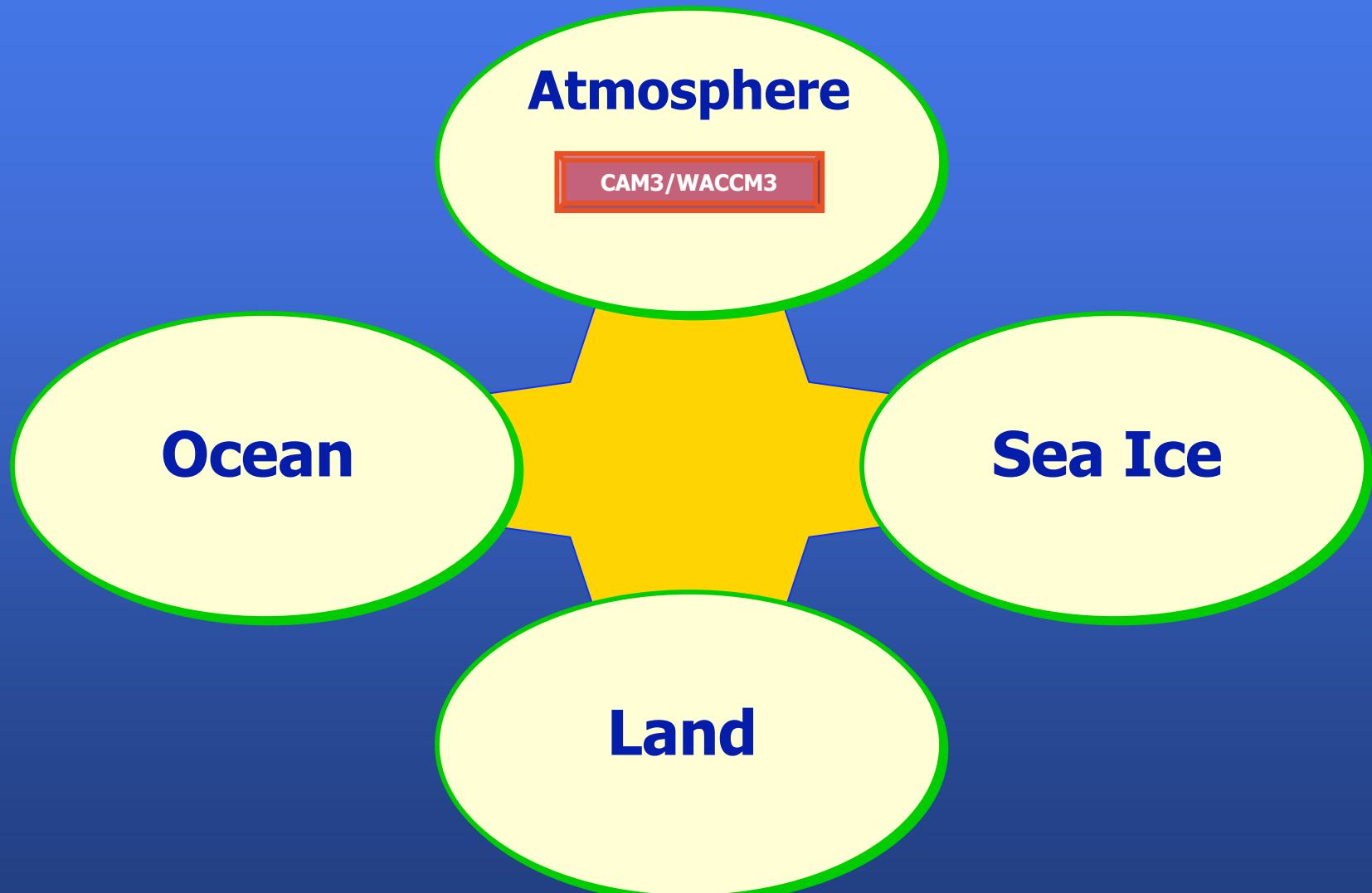
17 November 2004



# Global 3D Chemical Modeling at NCAR



# Community Climate System Model



# **WACCM Investigators**

- ACD: Rolando Garcia (PI)**

- Doug Kinnison, Dan Marsh, Stacy Walters, JF Lamarque, Aimee Merkel, Jaga Beres, Katj Mathis
- Bill Randel, Mijeong Park, Laura Pan, Cyndi Nevison, Louisa Emmons, Peter Hess, Anne Smith

- CGD: Byron Boville (PI)**

- Fabrizio Sassi, Andrew Gettelman
- Phil Rasch, Bill Collins, and many CAM3 colleagues etc...

- HAO: Ray Roble (PI)**

- Stan Solomon, Liying Qian, Art Richmond, Maura Hagan, Hanli Lui, Ben Foster

- LASP / CU**

- Cora Randall, Brian Toon, Glen Stewart, Mike Mills, Lynn Harvey, Cynthia Singleton, Chuck Bardeen.

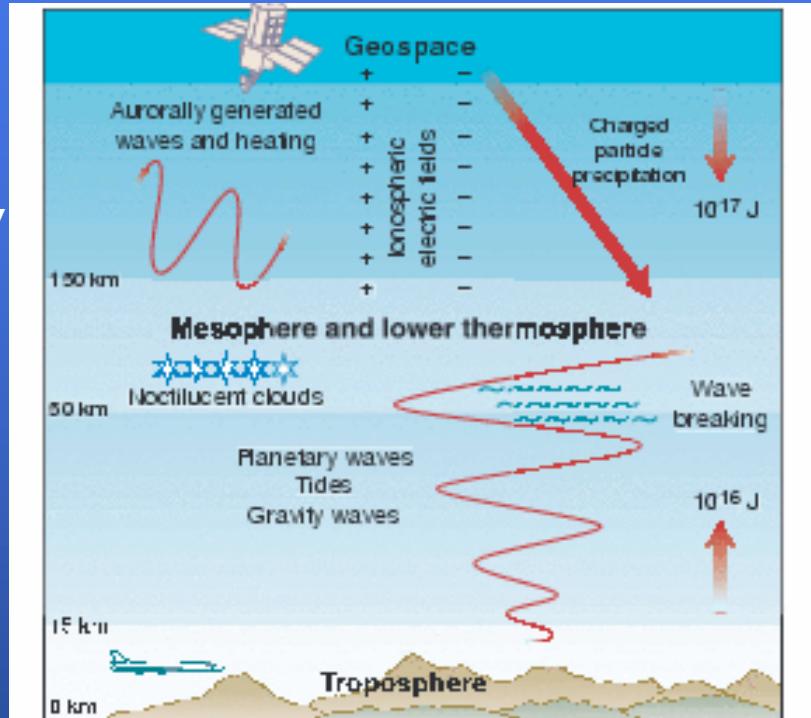
- University of Maryland.**

- Andy Dessler

# WACCM Motivation

(Roble, Geophysical Monographs, 123, 53, 2000)

- **Coupling between atmospheric layers:**
  - Waves transport energy and momentum from the lower atmosphere to drive the QBO, SAO, sudden warmings, mean meridional circulation
  - Solar inputs, e.g., auroral production of NO in the mesosphere and downward transport to the stratosphere
  - Stratosphere-troposphere exchange
- **Climate Variability and Climate Change:**
  - What is the impact of the stratosphere on tropospheric variability, e.g., the Arctic oscillation or “annular mode”?
  - How important is coupling among radiation, chemistry, and circulation? (e.g., in the response to O<sub>3</sub> depletion or CO<sub>2</sub> increase)

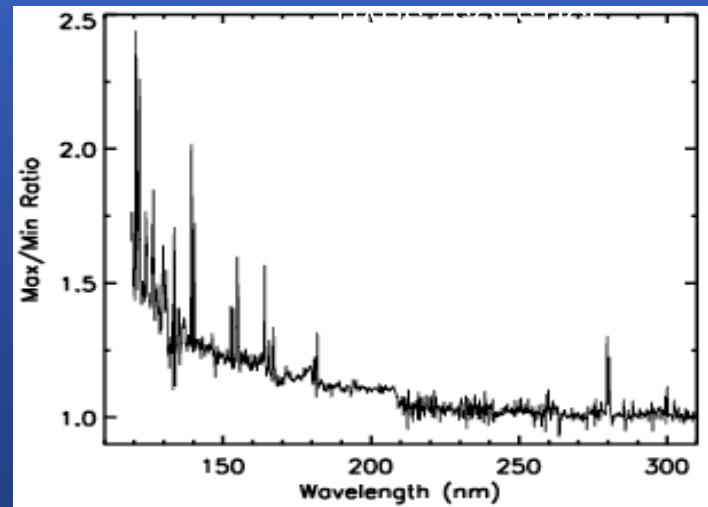
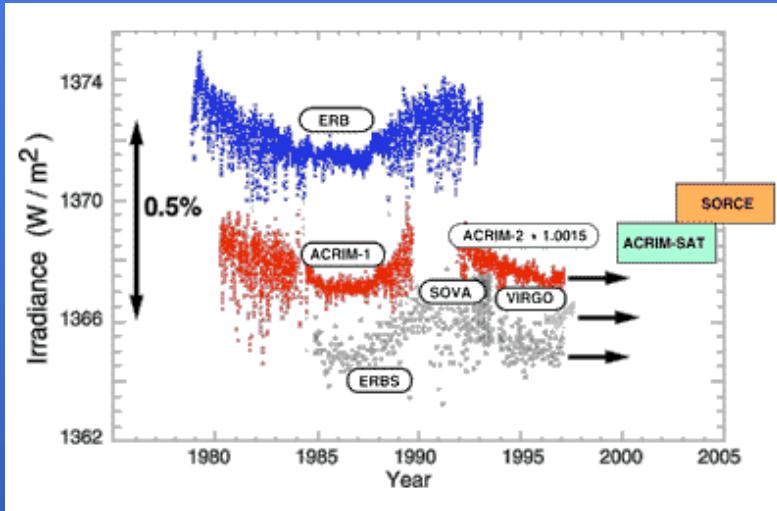


Energy transfer in the mesosphere and lower thermosphere. About  $10^{16} \text{ J}$  of energy propagates up daily from the atmosphere below in the form of waves and tides. During a geomagnetic storm (which occurs about every 5 days), about  $10^{17} \text{ J}$  is injected per day from space through auroral processes.

Jarvis, “Bridging the Atmospheric Divide”  
Science, 293, 2218, 2001

# WACCM Motivation

- Response to Solar Variability:
  - Recent satellite observations have shown that solar cycle variation is:
    - 0.1% for total Solar Irradiance
    - 5-10% at  $\approx 200\text{nm}$
  - Radiation at wavelengths near 200 nm is absorbed in the stratosphere  
=> Impacts on global climate may be mediated by stratospheric chemistry and dynamics
- Satellite observations:
  - There are several satellite programs that can benefit from a comprehensive model to help interpret observations
    - e.g., UARS, TIMED, EOS Aura



**Describe Model Components**

**Evaluation with Observations**

**H<sub>2</sub>O trend results**

**Discuss future direction**

# Extending the Community Atmospheric Model

## To form WACCM...

- Extended model from 85 - 150 km (66 lev; 1.3km lower strat to 3km in thermosphere)
- Parameterization of non-LTE IR (15  $\mu\text{m}$  band of CO<sub>2</sub> above 70 km) merged with CCSM IR parameterization (below 70 km)
- Short wave heating rates due to absorption of radiation shortward of 200 nm and chemical potential heating
- Gravity Wave parameterization extended upward, includes dissipation by molecular viscosity
- Diffusive separation of atmospheric constituents above about 90 km
- Modified cloud water and near-IR parameterizations for more accurate seasonal cycle of temperature at tropopause
- Finite-volume dynamics (Lin and Rood, 1996) - WACCM3
  - Semi-Lagrangian dynamics - WACCM1b

# Model Chemistry - 50 Species Mechanism

**Long-lived Species:** (19-species) - Explicit Forward Euler

Misc:	CO <sub>2</sub> , CO, CH <sub>4</sub> , H <sub>2</sub> O, N <sub>2</sub> O, H <sub>2</sub> , O <sub>2</sub>
CFCs:	CCl <sub>4</sub> , CFC-11, CFC-12, CFC-113
HCFCs:	HCFC-22
Chlorocarbons:	CH <sub>3</sub> Cl, CH <sub>3</sub> CCl <sub>3</sub> ,
Bromocarbons:	CH <sub>3</sub> Br
Halons:	H-1211, H-1301
Constant Species:	N <sub>2</sub> , N( <sup>2</sup> D)

**Short-lived Species:** (31-species) - Implicit Backward Euler\*

O <sub>x</sub> :	O <sub>3</sub> , O, O( <sup>1</sup> D)
NO <sub>x</sub> :	N, NO, NO <sub>2</sub> , NO <sub>3</sub> , N <sub>2</sub> O <sub>5</sub> , HNO <sub>3</sub> , HO <sub>2</sub> NO <sub>2</sub>
ClO <sub>x</sub> :	Cl, ClO, Cl <sub>2</sub> O <sub>2</sub> , OCLO, HOCl, HCl, ClONO <sub>2</sub> , Cl <sub>2</sub>
BrO <sub>x</sub> :	Br, BrO, HOBr, HBr, BrCl, BrONO <sub>2</sub>
HO <sub>x</sub> :	H, OH, HO <sub>2</sub> , H <sub>2</sub> O <sub>2</sub>
CH <sub>4</sub> derivatives:	CH <sub>2</sub> O, CH <sub>3</sub> O <sub>2</sub> , CH <sub>3</sub> OOH

\* Non-linear system of equations are solved using a Newton Raphson iteration technique; uses sparse matrix techniques; Sandu et al, *J. Comp. Phys.*, 129, 101-110, 1996.

# **Model Chemistry - 106 Species Mechanism**

**(219 Thermal; 18 Het.; 71 photolytic)**

## **Additional Surface Source Gases (13 additional) ...**

NHMCs:             $\text{CH}_3\text{OH}$ ,  
 $\text{C}_2\text{H}_6$ ,  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_5\text{OH}$ ,  $\text{CH}_3\text{CHO}$   
 $\text{C}_3\text{H}_8$ ,  $\text{C}_3\text{H}_6$ ,  $\text{CH}_3\text{COCH}_3$  (Acetone)  
 $\text{C}_4\text{H}_8$  (BIGENE),  $\text{C}_4\text{H}_8\text{O}$  (MEK)  
 $\text{C}_5\text{H}_8$  (Isoprene),  $\text{C}_5\text{H}_{12}$  (BIGALK)  
 $\text{C}_7\text{H}_8$  (Toluene)  
 $\text{C}_{10}\text{H}_{16}$  (Terpenes)

Radicals:           Approx. 45 additional species.

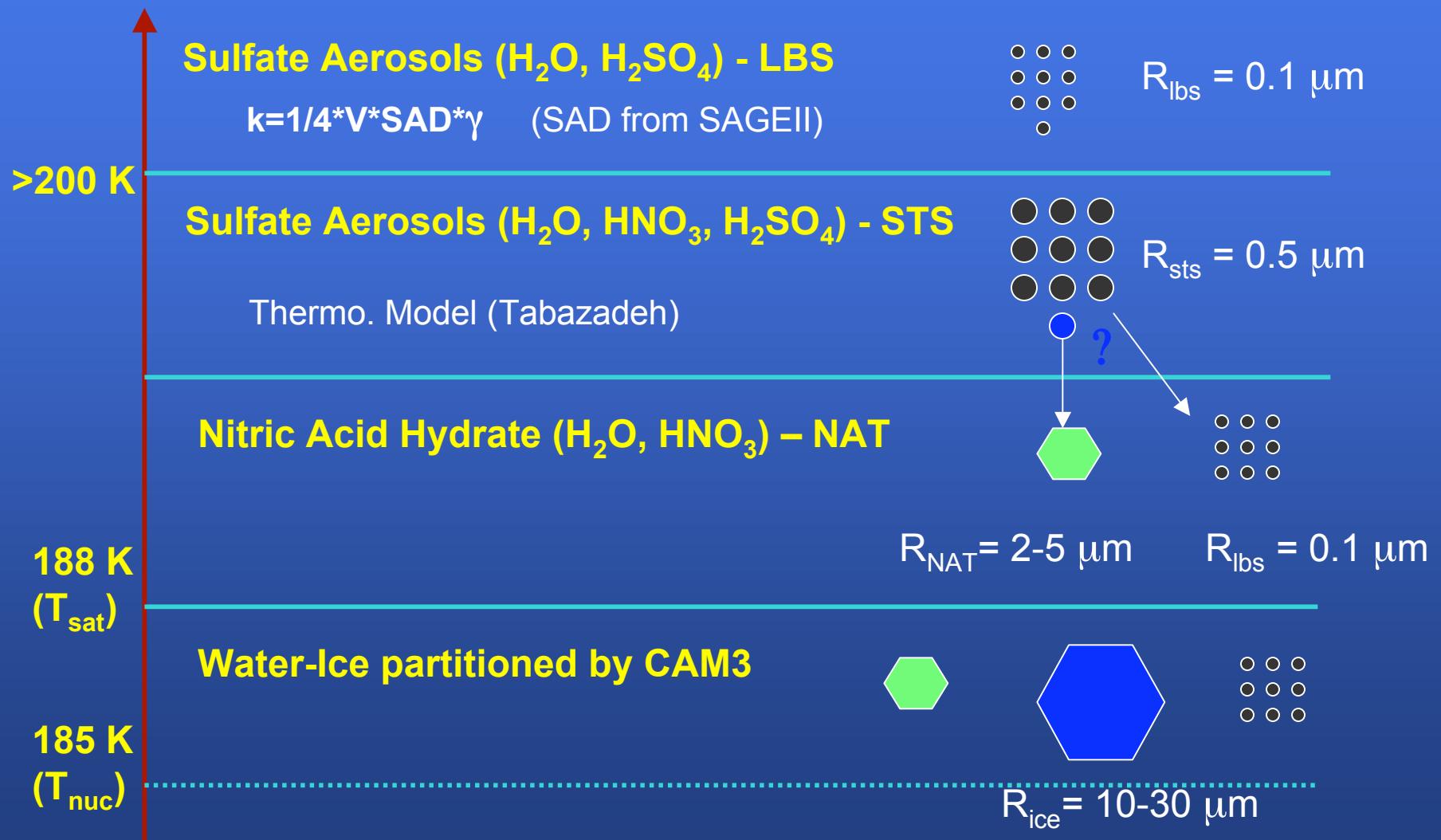
**Include:**           Detailed 3D (lat/lon/time) emission inventories of natural and anthropogenic surface sources

Dry and wet deposition of soluble species  
Lightning and Aircraft production of NOx

More information: JF Larmarque, P. Hess, L. Emmons.

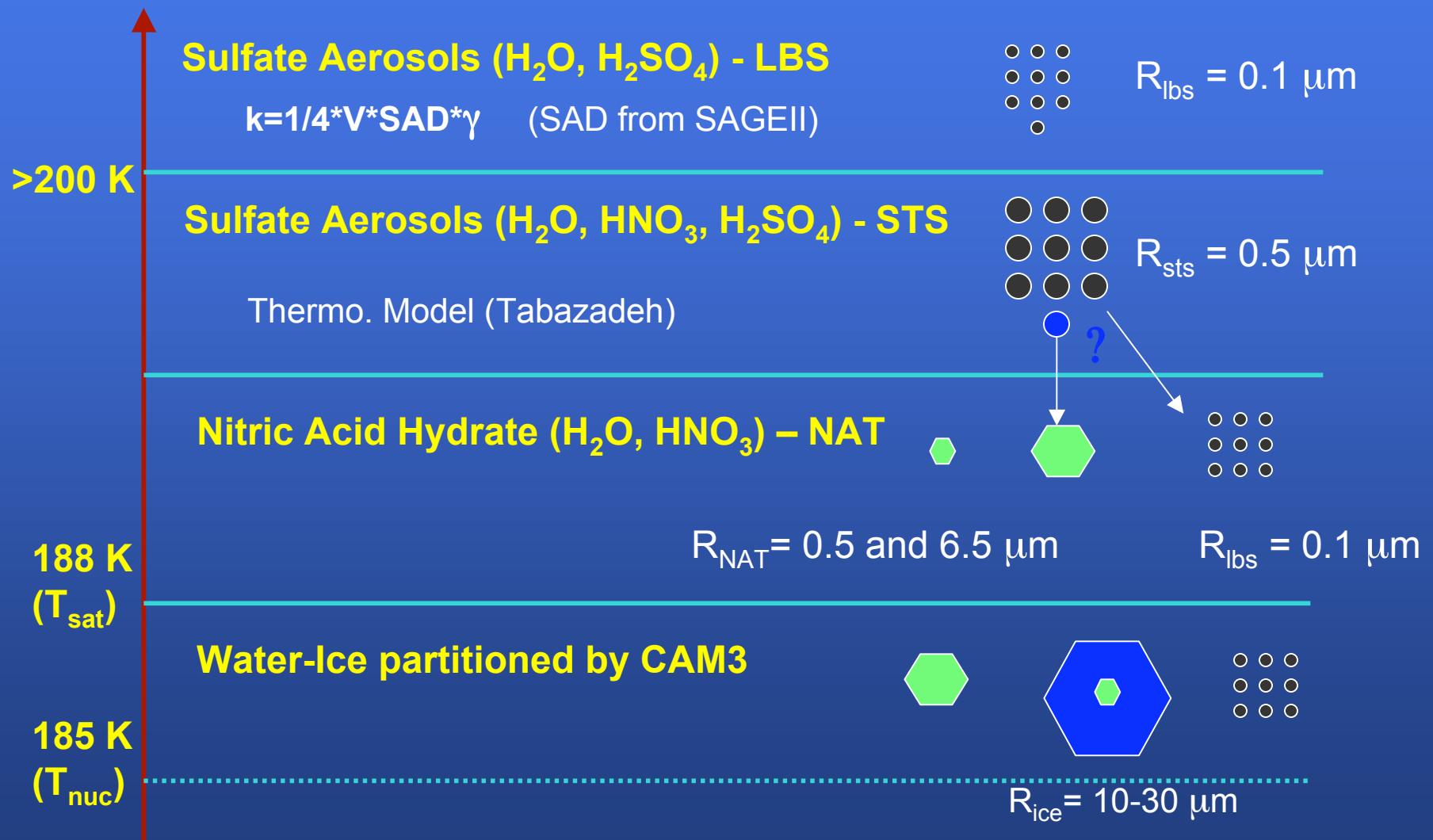
# Model Chemistry (1) - Heterogeneous Processes

Considine et. al., JGR, 2000



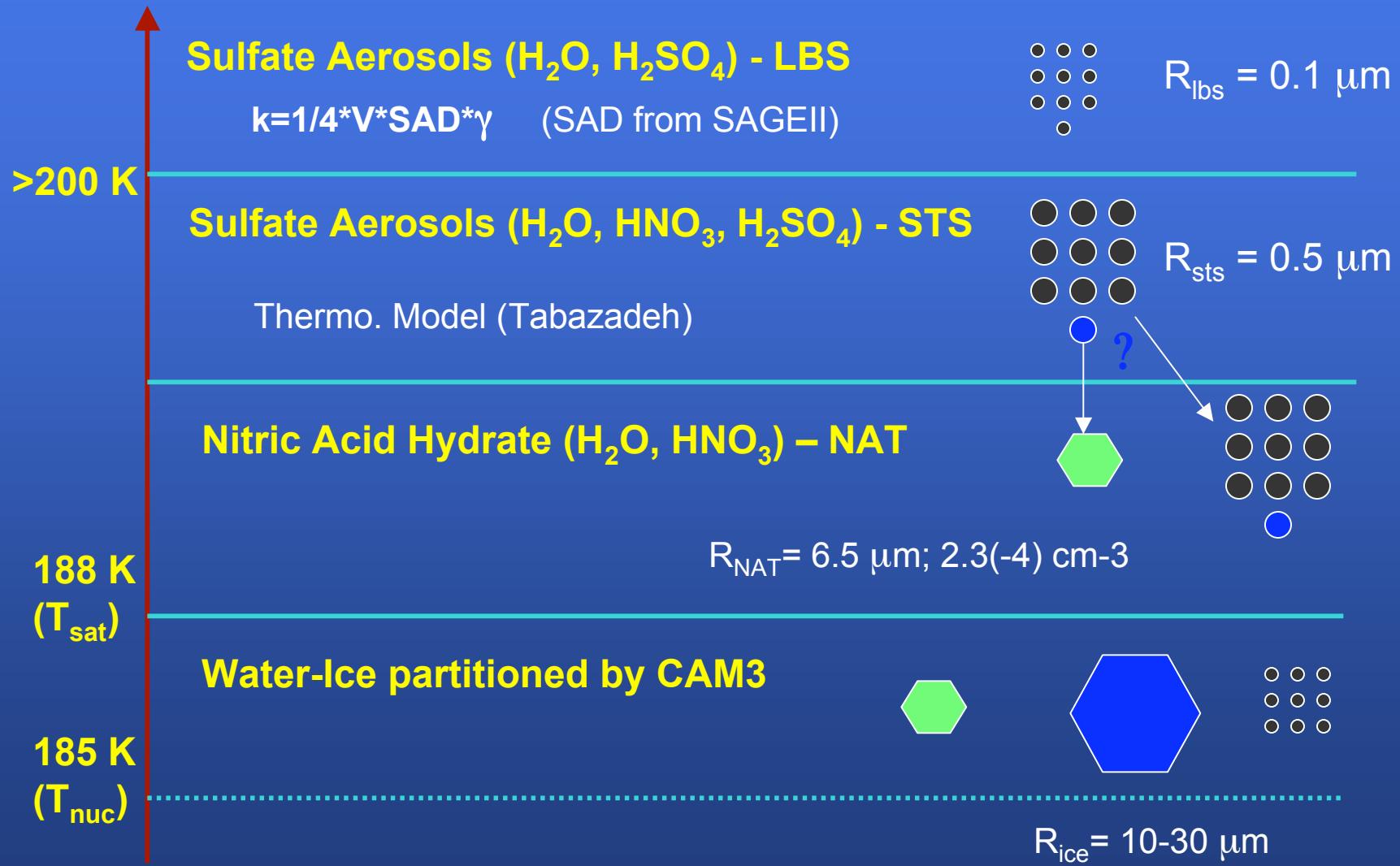
## Model Chemistry (2) - Heterogeneous Processes

Considine, +Davies, JGR, 108, 832, 2003.



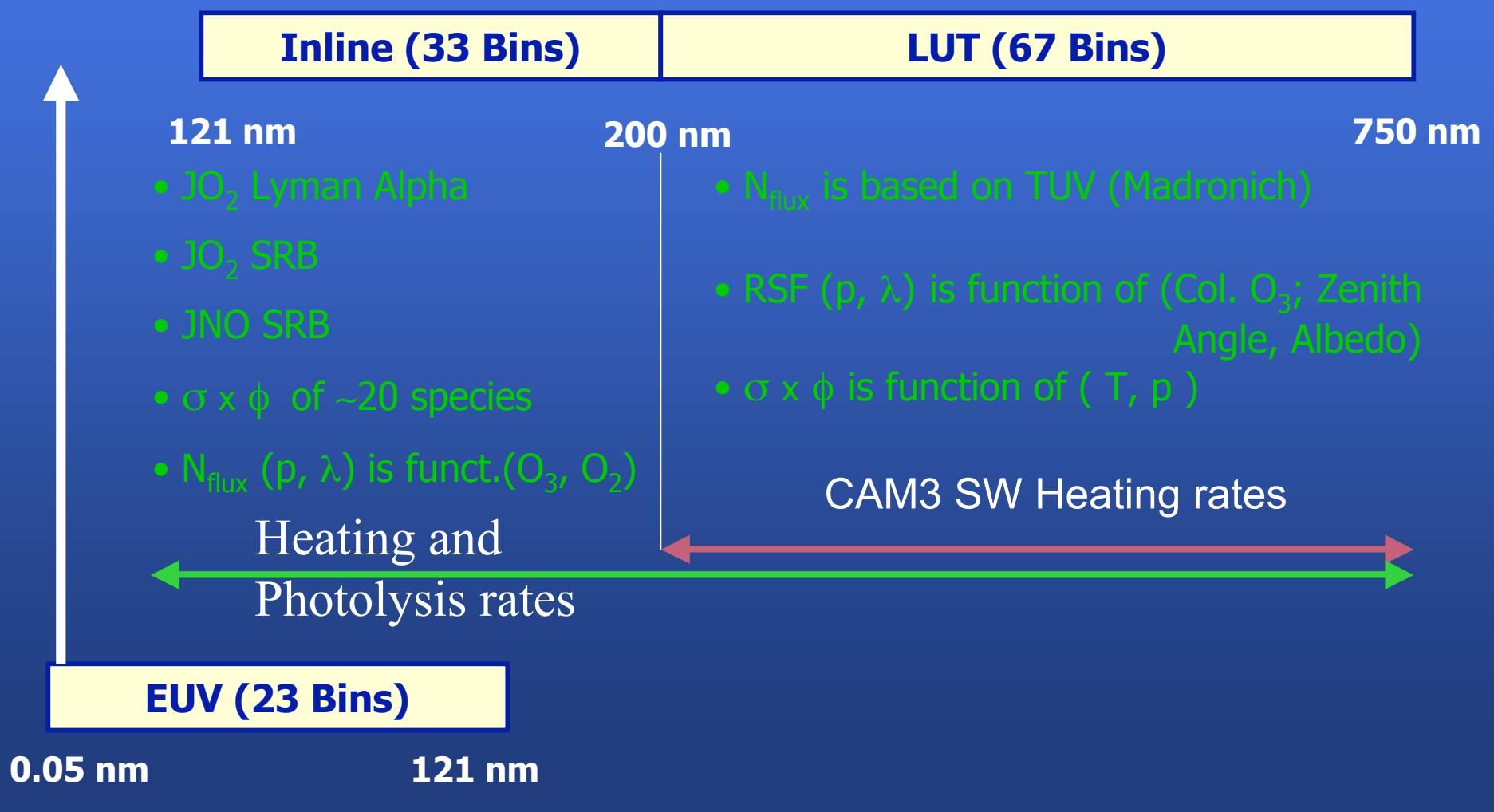
# Model Chemistry (3) - Heterogeneous Processes

Considine, +Drdla et al., JGR, 108, 8318, 2003.



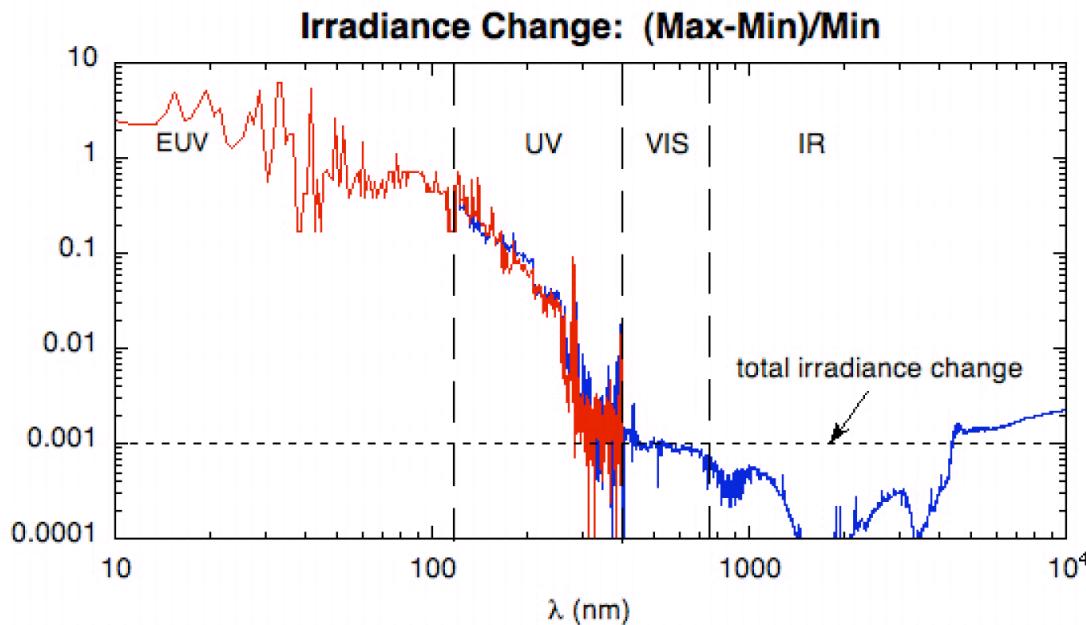
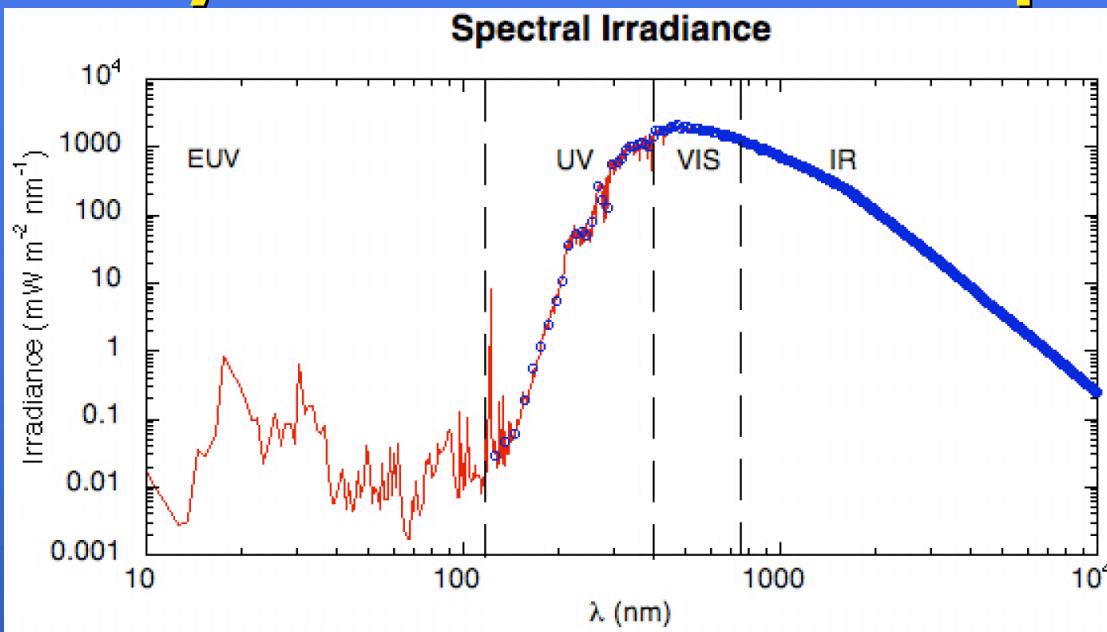
# Model Chemistry - Photolytic Processes

$$J_{O_2}(p) = \sum F_{\text{exo}}(\lambda, t) \times N_{\text{flux}}(p, \lambda) \times \sigma(\lambda) \times \phi(\lambda)$$



# Solar Cycle Studies: Model Input

Spectral composite  
courtesy of:  
Judith Lean (NRL)  
and  
Tom Woods (CU/LASP)



# E-Region Ion Chemistry Included in WACCM2

Ion species:

$\text{N}_2^+$ ,  $\text{O}_2^+$ ,  $\text{N}^+$ ,  $\text{O}^+$ ,  $\text{NO}^+$ , and  $e^-$

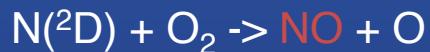
Photon / Photoelectron processes with  
 $\text{O}$ ,  $\text{N}$ ,  $\text{O}_2$ ,  $\text{N}_2$

Approx. 25 reactions...

reactions:

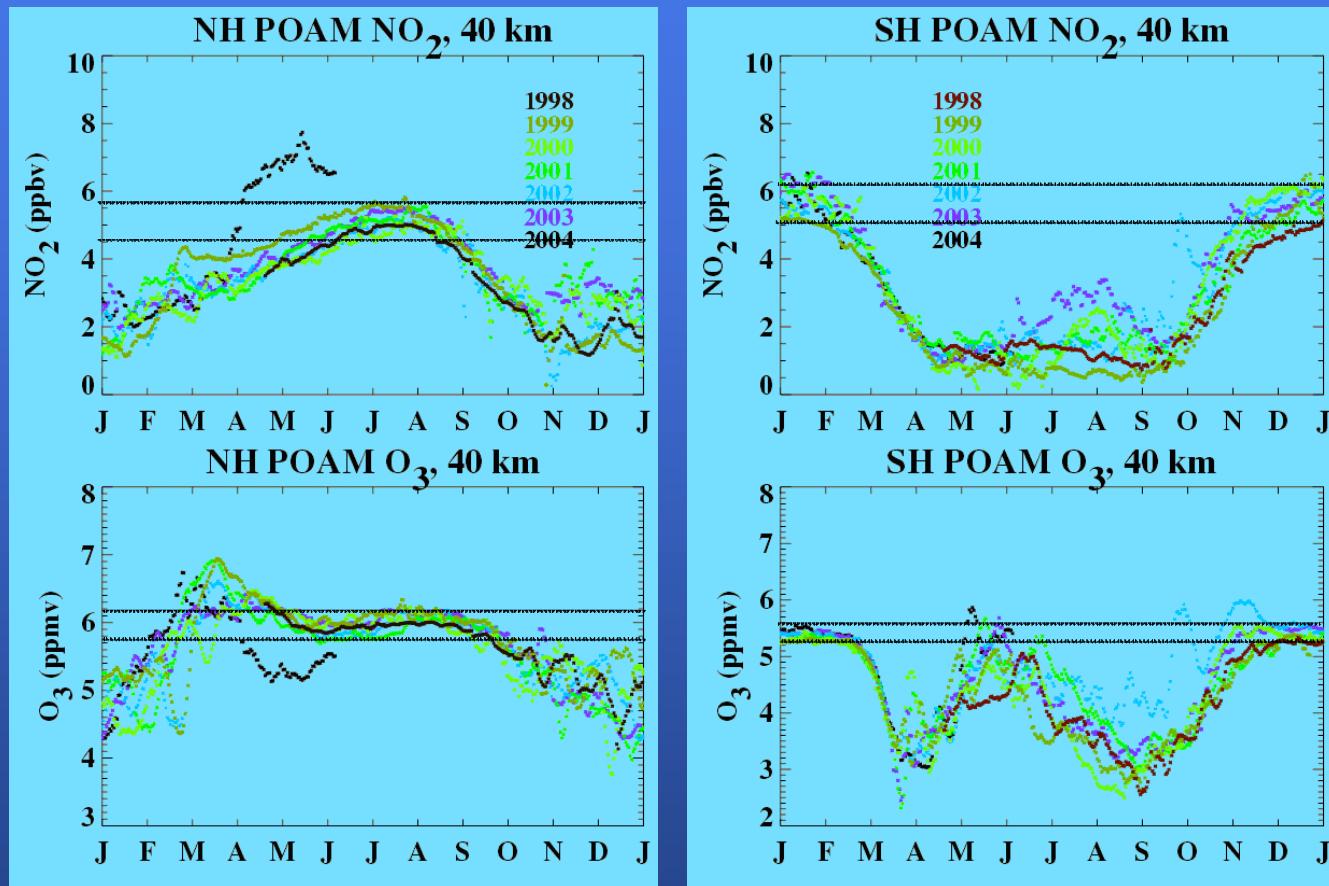
- r1:  $\text{O}^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{O}$
- r2:  $\text{O}^+ + \text{N}_2 \rightarrow \text{NO}^+ + \text{N}$
- r3:  $\text{N}_2^+ + \text{O} \rightarrow \text{NO}^+ + \text{N}(^2\text{D})$
- r4:  $\text{O}_2^+ + \text{N} \rightarrow \text{NO}^+ + \text{O}$
- r5:  $\text{O}_2^+ + \text{NO} \rightarrow \text{NO}^+ + \text{O}_2$
- r6:  $\text{N}^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{N}$
- r7:  $\text{N}^+ + \text{O}_2 \rightarrow \text{NO}^+ + \text{O}$
- r8:  $\text{N}^+ + \text{O} \rightarrow \text{O}^+ + \text{N}$
- r9:  $\text{N}_2^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{N}_2$
- r10:  $\text{O}_2^+ + \text{N}_2 \rightarrow \text{NO}^+ + \text{NO}$
- r11:  $\text{N}_2^+ + \text{O} \rightarrow \text{O}^+ + \text{N}_2$

- ra1:  $\text{NO}^+ + e^- \rightarrow \text{N} + \text{O}$  (20%)  
->  $\text{N}(^2\text{D}) + \text{O}$  (80%)
- ra2:  $\text{O}_2^+ + e^- \rightarrow 2\text{O}$  (15%)  
->  $\text{O}(^1\text{D}) + \text{O}$  (85%)
- ra3:  $\text{N}_2^+ + e^- \rightarrow 2\text{N}$  (10%)  
->  $\text{N}(^2\text{D}) + \text{N}$  (90%)



Courtesy of D. Marsh

**Interannual variability in POAM  $\text{NO}_2$  exceeds 15% even in summer; Variability in summertime Ozone ~5-7%.**

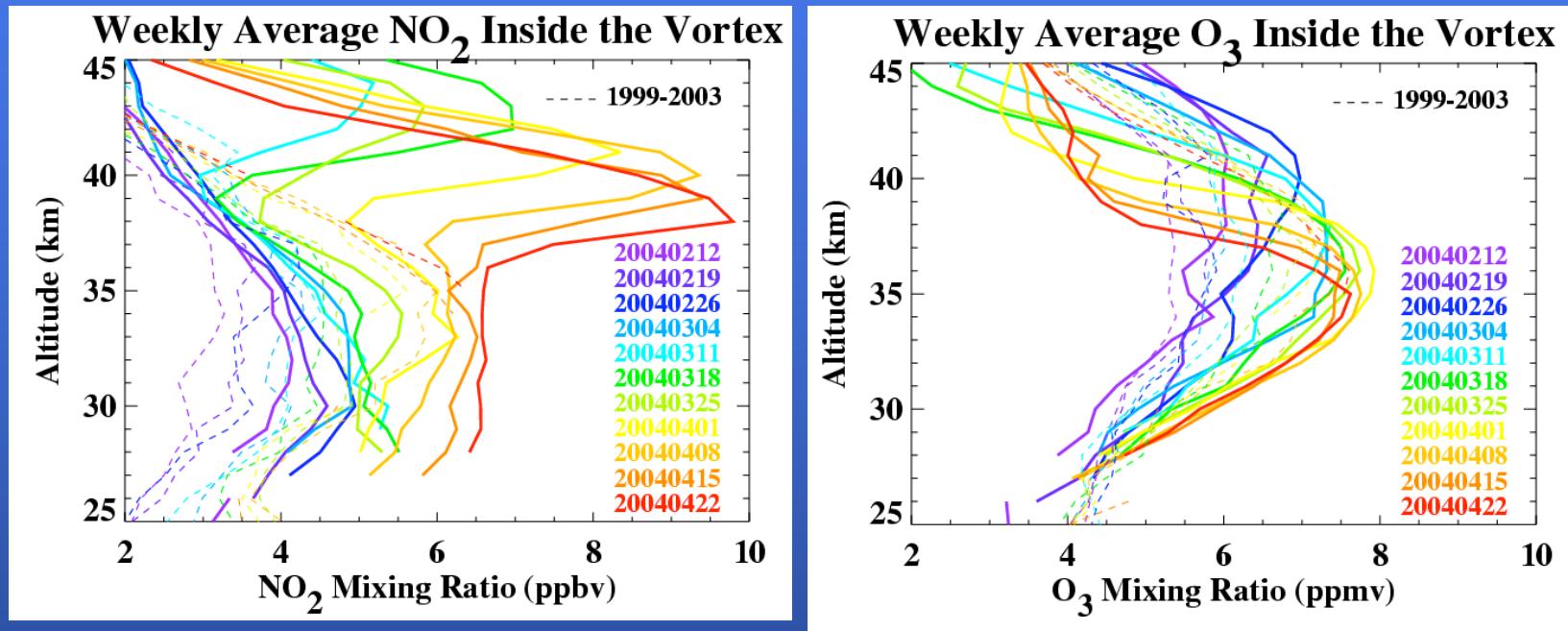


Some of the variability can be attributed to **ENERGETIC PARTICLE EFFECTS**.

How significant are the errors in 3D simulations and trend analyses when energetic particle effects are ignored?

Courtesy of Cora Randall

# Unprecedented high $\text{NO}_2$ descends inside the NH vortex in Mar-Apr 2004: Corresponds to unprecedented low $\text{O}_3$



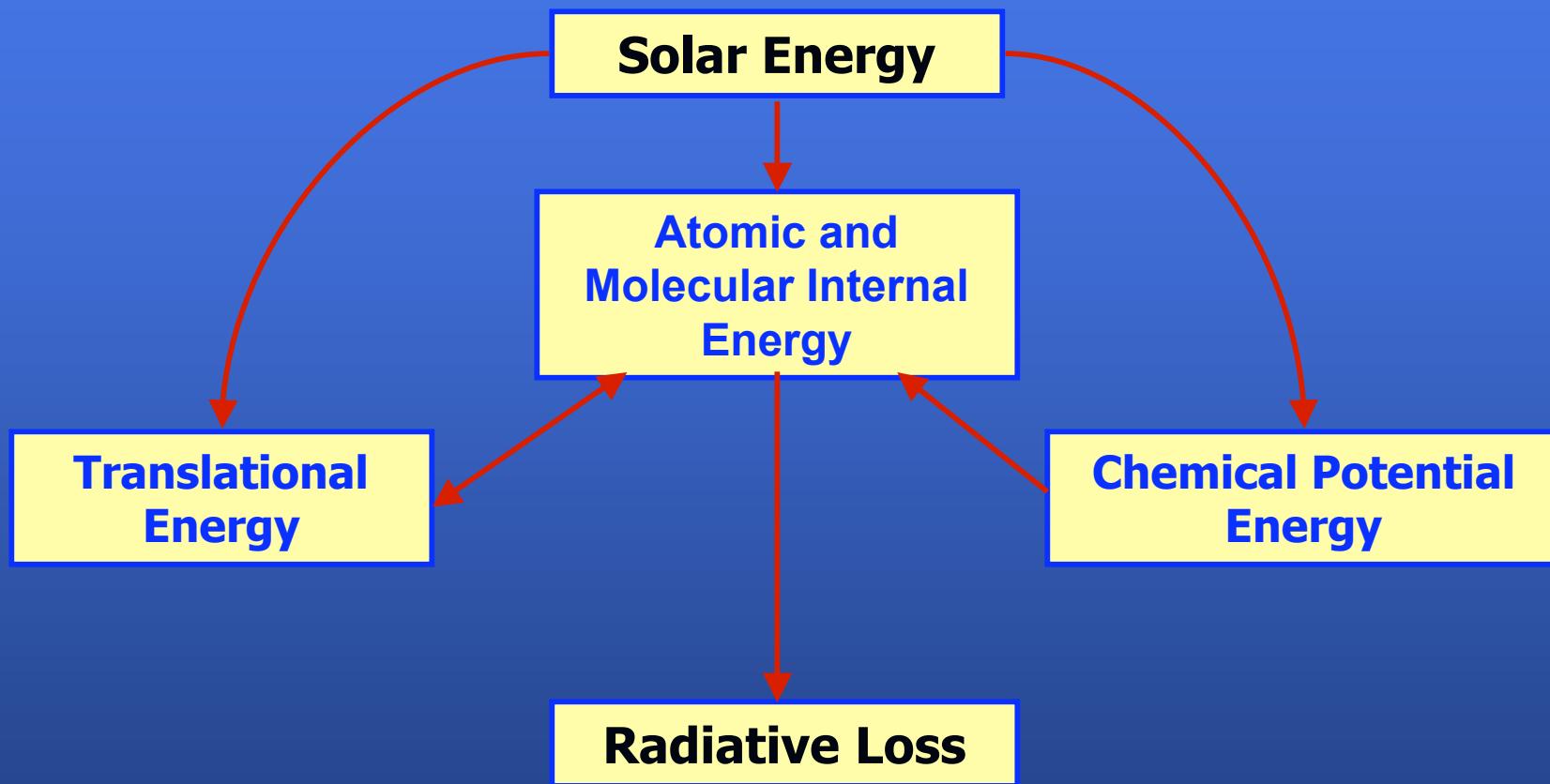
Solid lines: Weekly averages in 2004

Dotted lines: Weekly averages including data from 1999-2003

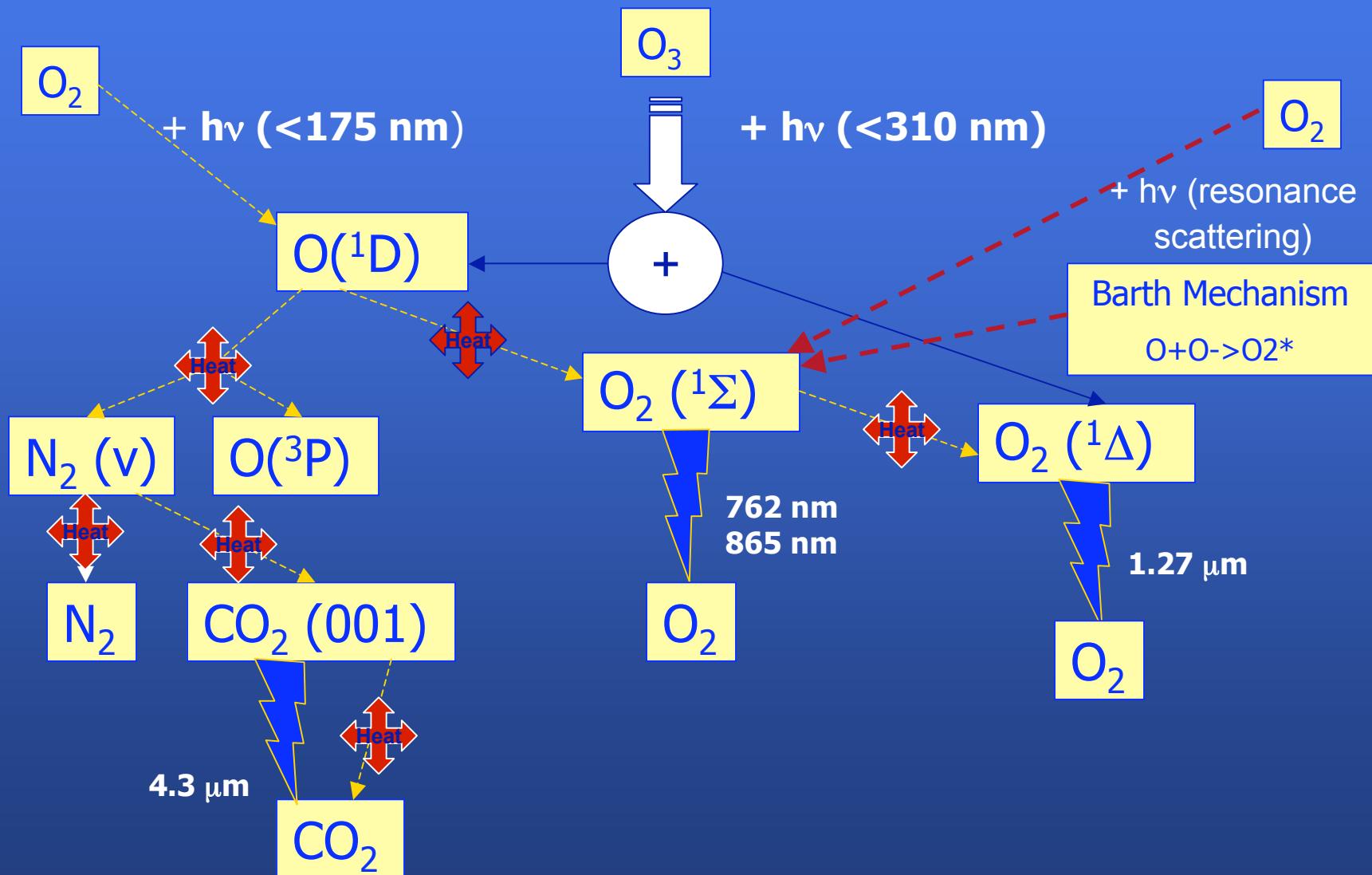
$\text{NO}_x$  enhancements and  $\text{O}_3$  decreases are due to **ENERGETIC PARTICLE PRODUCTION** of mesospheric  $\text{NO}$ , which descends to the stratosphere and catalytically destroys  $\text{O}_3$ .

Courtesy of Cora Randall

# Heating Rate Approach



# Heating Rate Approach Cont...

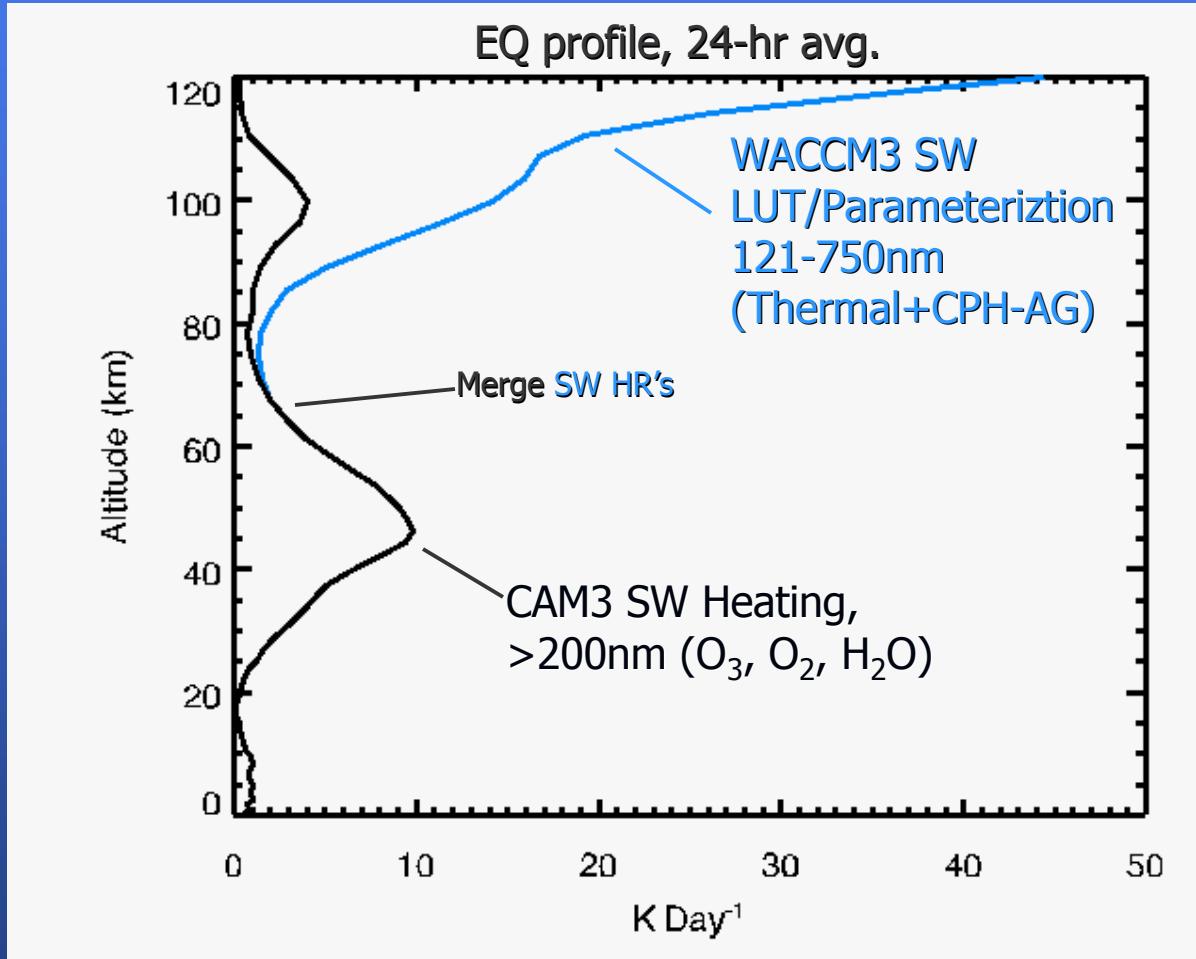


# Chemical Potential Heating

Chemical Reactions	Kcal/mole
$O + O_3 \Rightarrow 2O_2$	-93.65
$O + O + M \Rightarrow O_2 + M$	-119.40
$O + OH \Rightarrow H + O_2$	-16.77
$O + HO_2 \Rightarrow OH + O_2$	-53.27
$H + O_2 + M \Rightarrow HO_2 + M$	-49.10
$O + O_2 + M \Rightarrow O_3 + M$	-25.47
$H + O_3 \Rightarrow OH + O_2$	-76.90
$HO_2 + NO \Rightarrow NO_2 + OH$	-7.83
$HO_2 + O_3 \Rightarrow OH + 2O_2$	-28.29
$HO_2 + HO_2 \Rightarrow H_2O_2 + O_2$	-39.58
$OH + O_3 \Rightarrow HO_2 + O_2$	-39.91
$NO + O_3 \Rightarrow NO_2 + O_2$	-47.74
$NO_2 + O \Rightarrow NO + O_2$	-45.91
$OH + HO_2 \Rightarrow H_2O + O_2$	-70.61
$H + HO_2 \Rightarrow H_2 + O_2$	-55.68

Mlynczak and Solomon

# Heating Rate Approach (WACCM2)



**Describe Model Components**

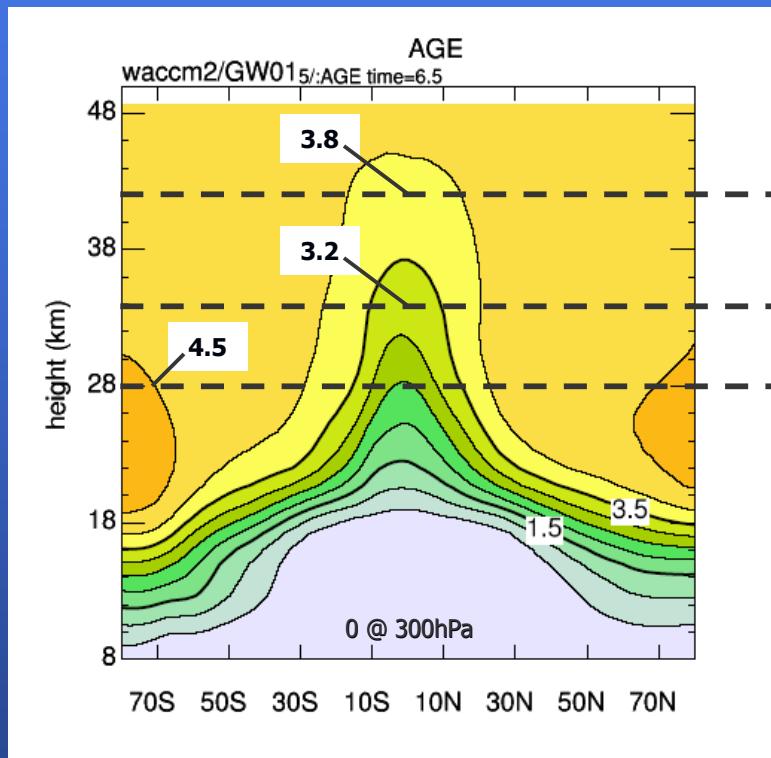
**Evaluation with Observations**

**H<sub>2</sub>O trend results**

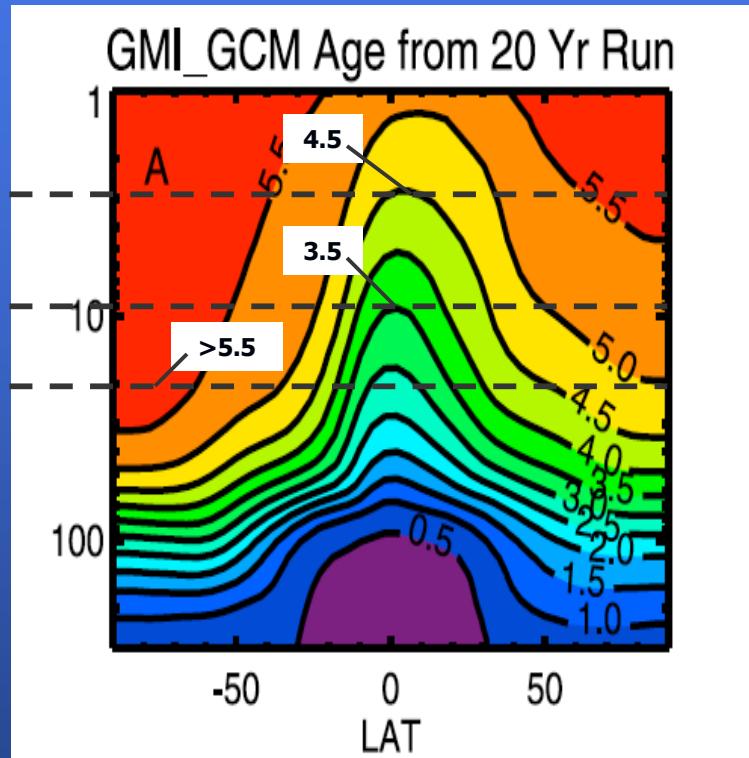
**Discuss future direction**

# Age-of-Air Comparison's

WACCM3



GMI/FVGCM



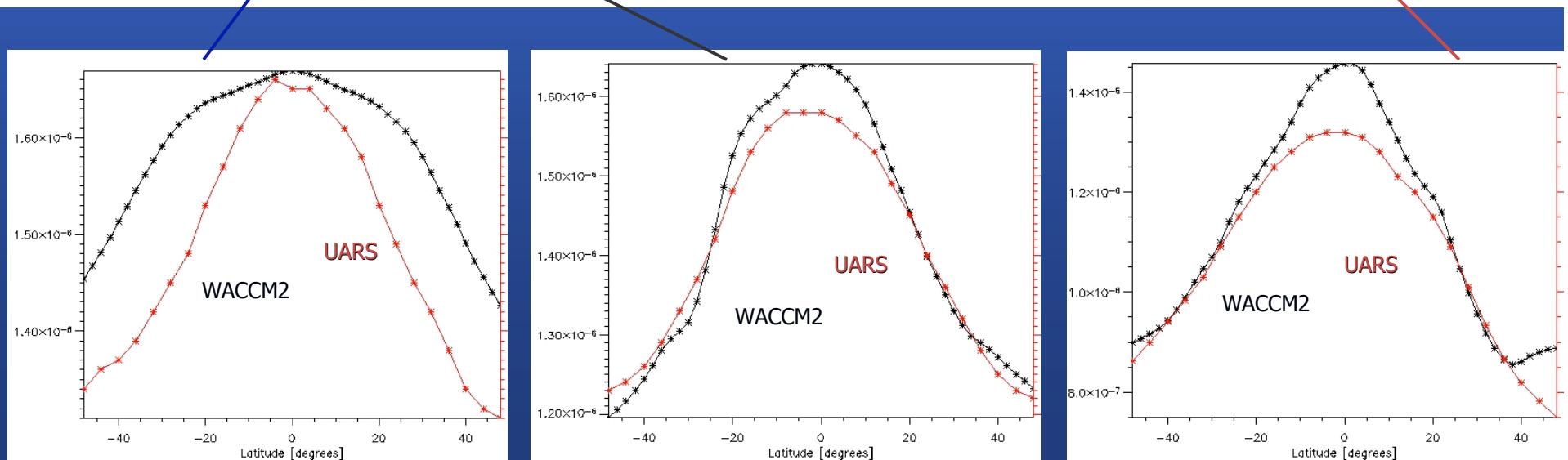
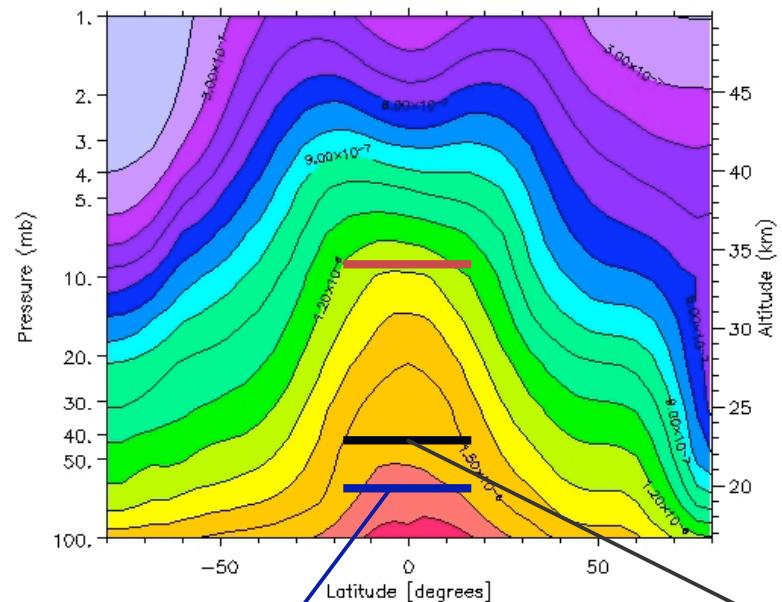
Sassi et al., 2004

Considine et al., JGR, 2004

# CH<sub>4</sub>, April

HALOE+CLAES Clim (Courtesy of B. Randel)

WACCM2



# Ozone Comparison with Occultation Climatology

L. Harvey and C. Randall,  
LASP

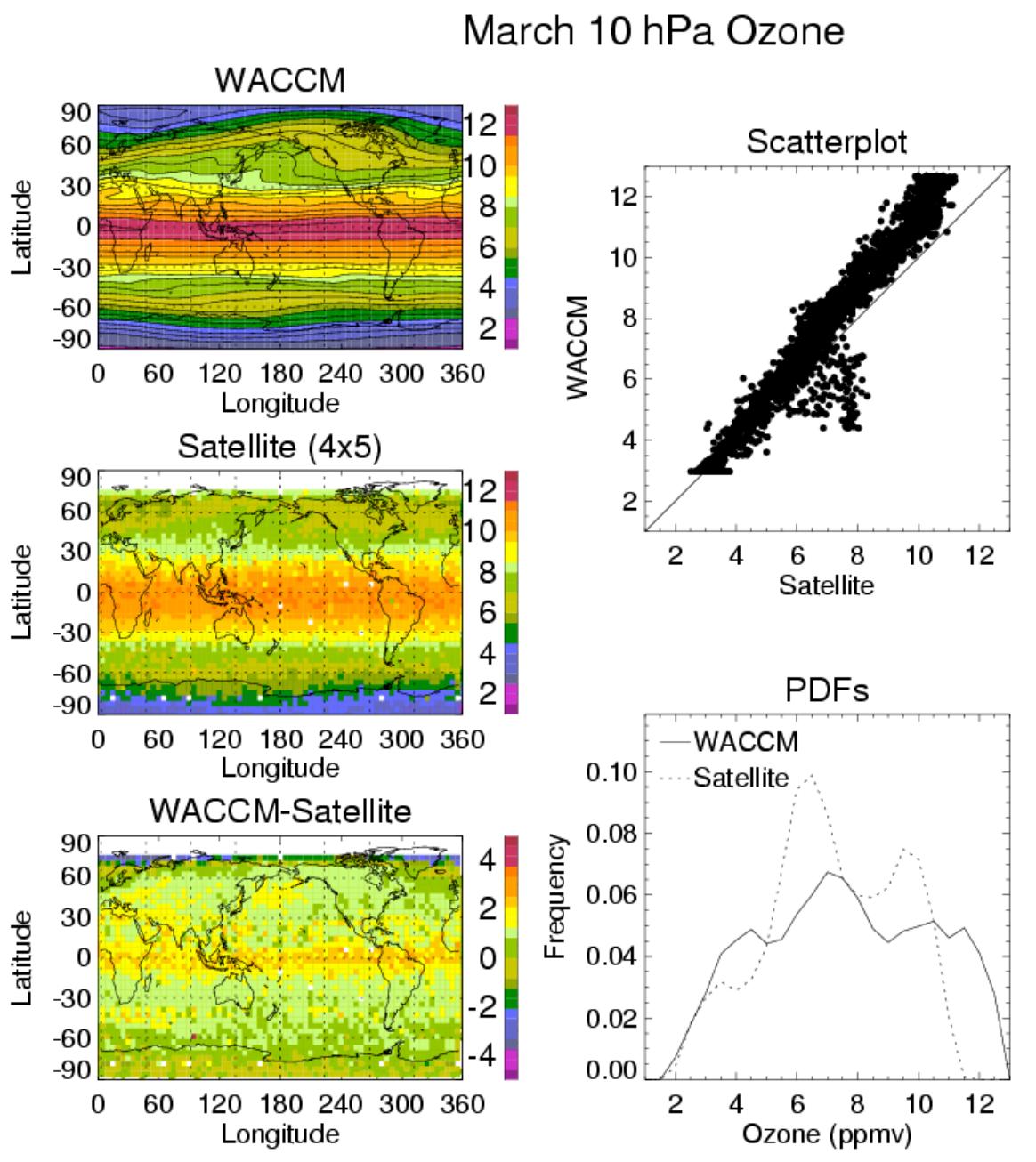
Monthly Mean Climatology  
 $4^{\circ}$  (longitude) x  $5^{\circ}$  (latitude) Grid

Occultation Data: SAGE II, III  
(1984-Present)

POAM II, III (1994-Present)

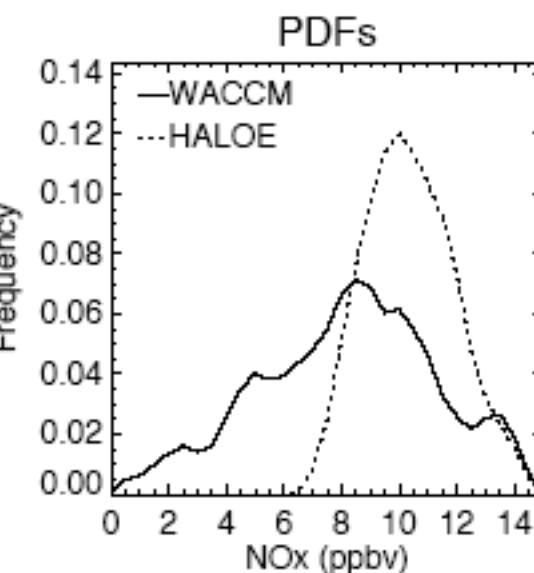
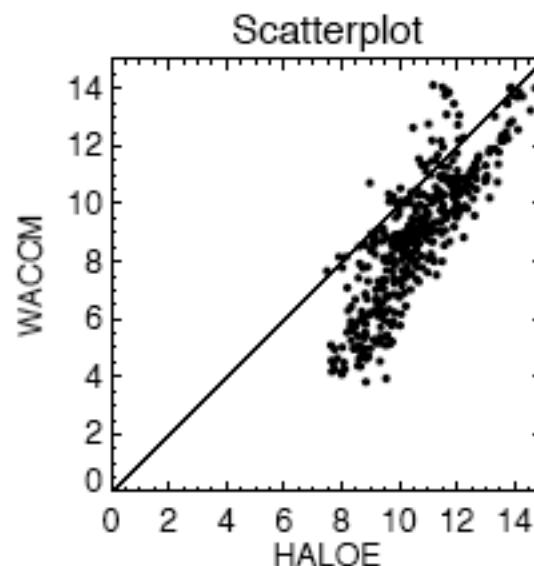
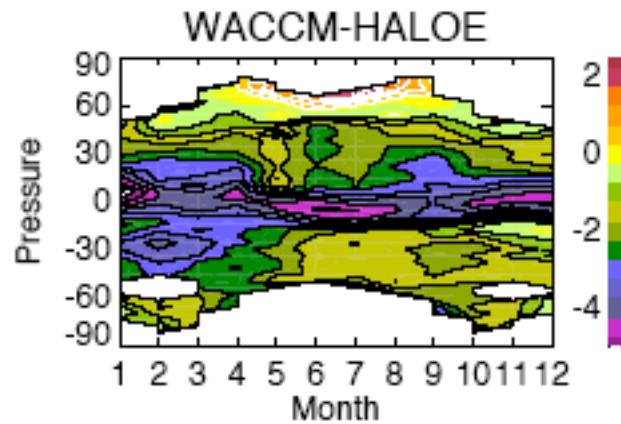
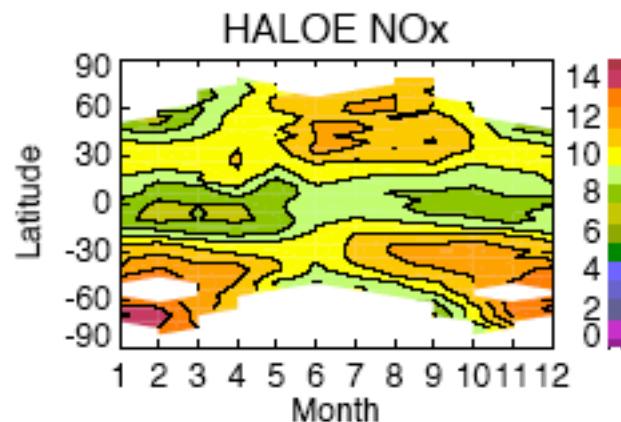
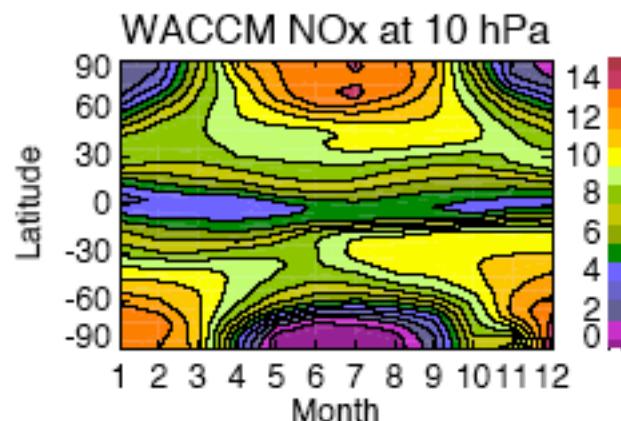
ILAS (1996-1997)

HALOE (1991-Present)



# NO<sub>x</sub>

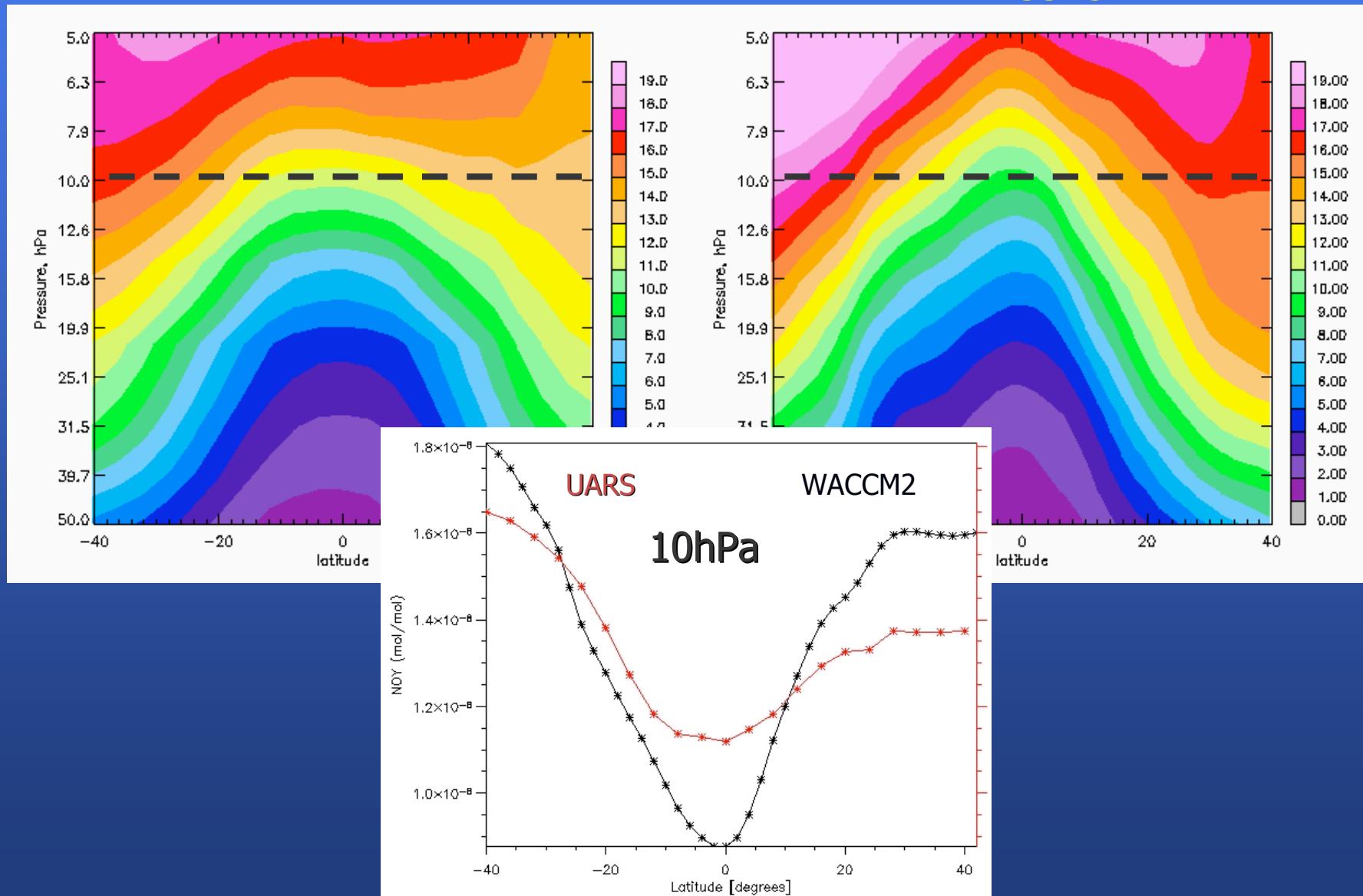
L. Harvey and C.  
Randall, LASP



# $\text{NO}_\text{Y}$ , April, Monthly Mean

UARS:  $\text{NO}_\text{x}$  HALOE+  $\text{HNO}_3$  CLAES

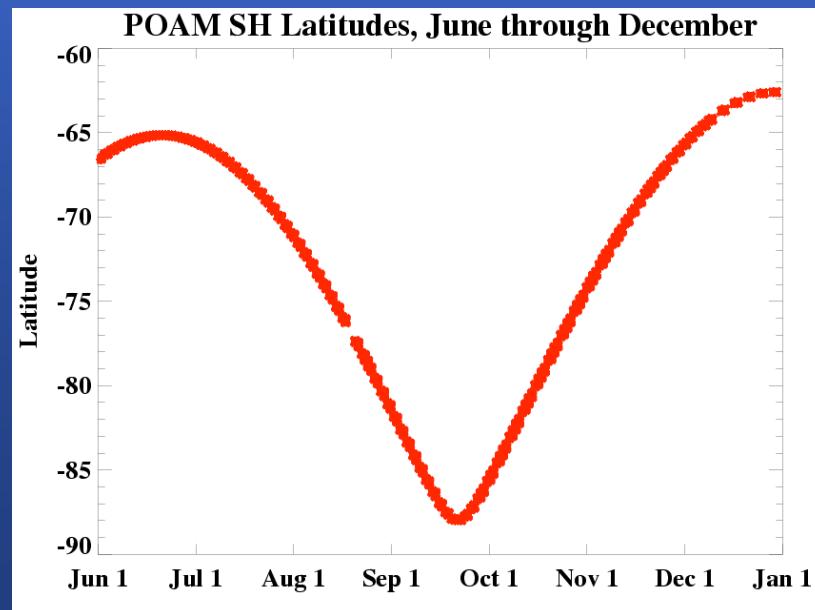
WACCM3

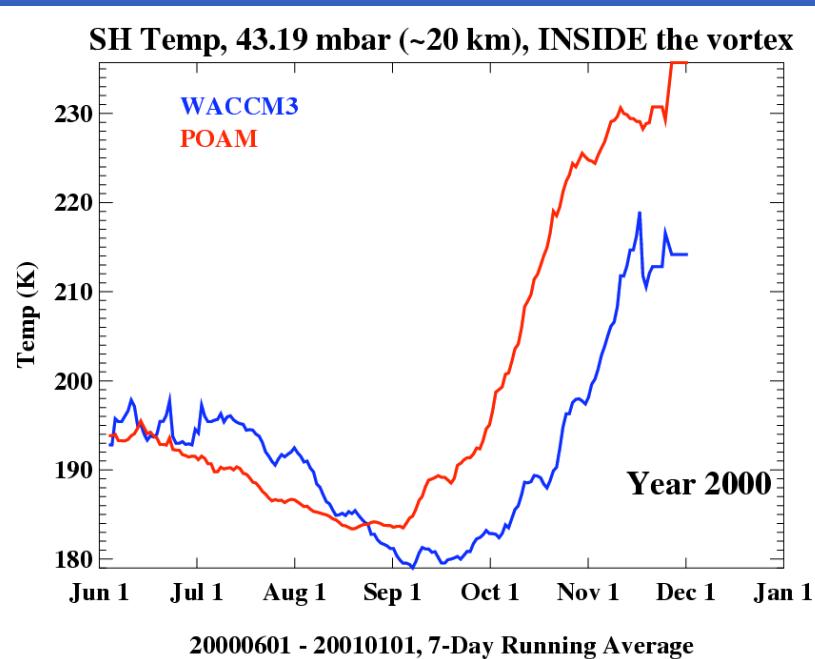
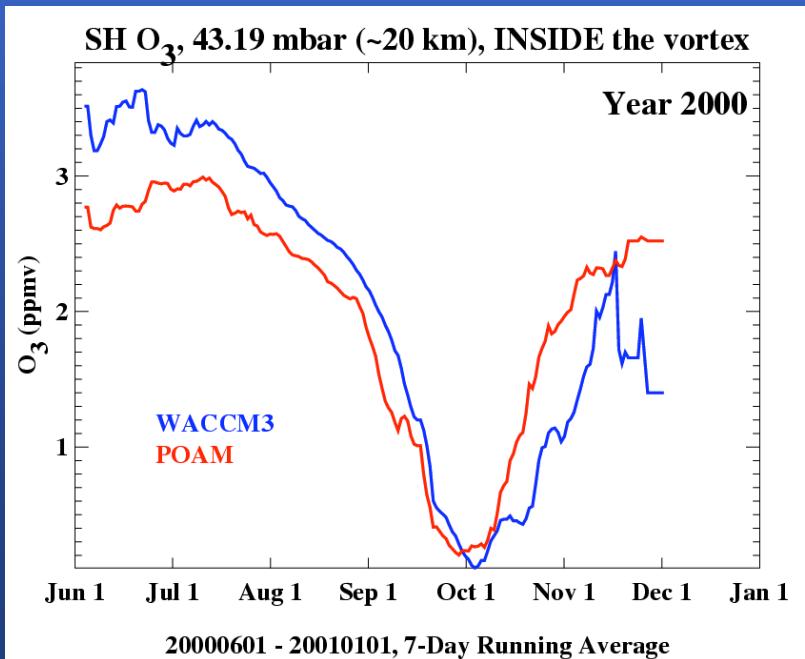
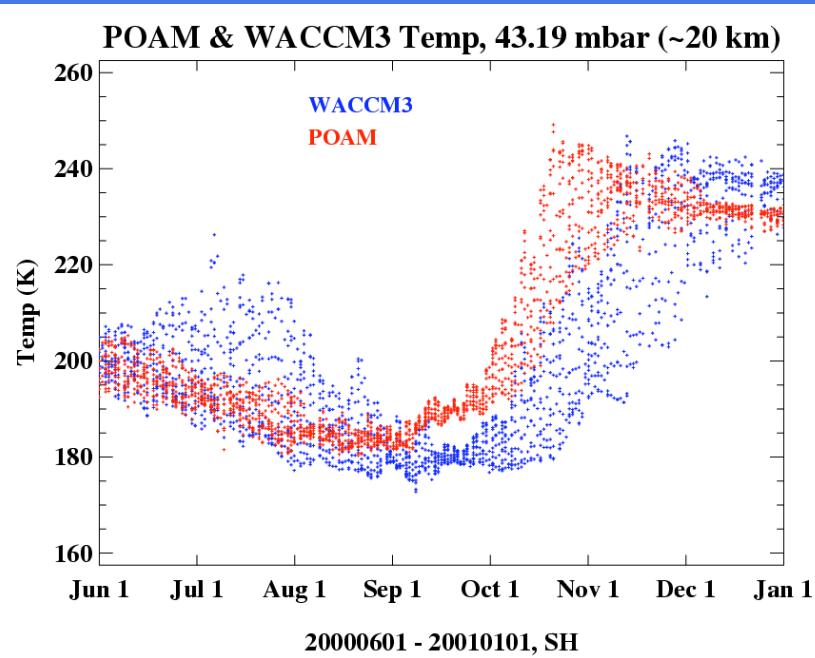
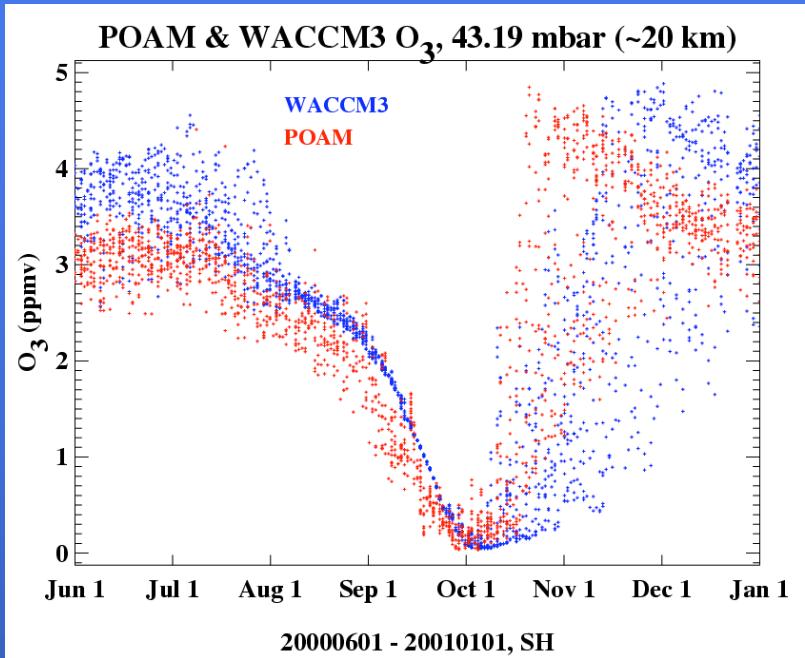


# Comparisons of Ozone and Temperature from POAM & WACCM3

- POAM data version 4.0, year 2000 (can easily do for other years)
- “POAM” Temperatures are actually UKMO
- WACCM3 file: T\_O3\_WACCM3\_ions\_photo\_v2.2.nc
- POAM data interpolated to WACCM3 pressure levels
- WACCM3 interpolated to POAM lat/lon

POAM latitude dependence (repeated annually):



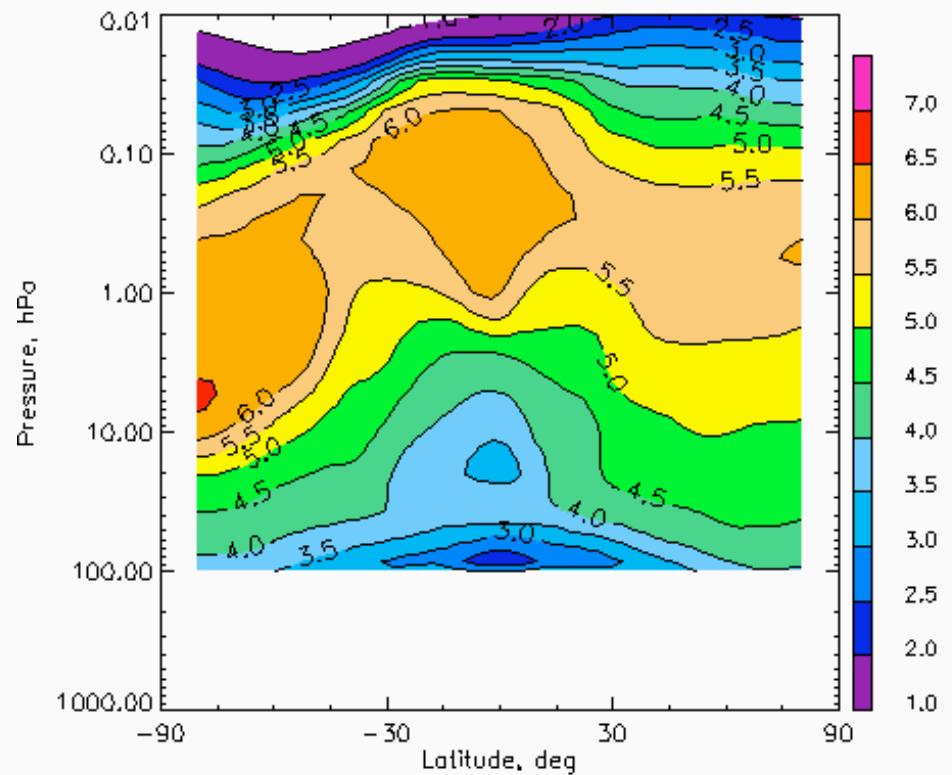
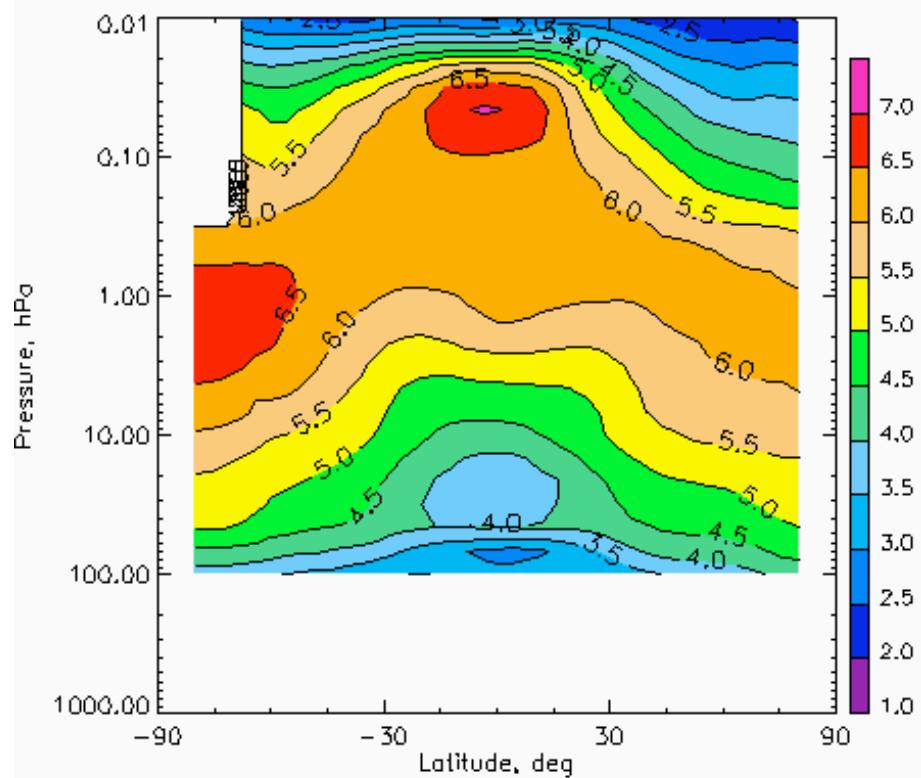


# $\text{H}_2\text{O}$ (WACCM2)

Stratosphere / Mesosphere Distribution \*\*\* May

HALOE/MLS

WACCM3



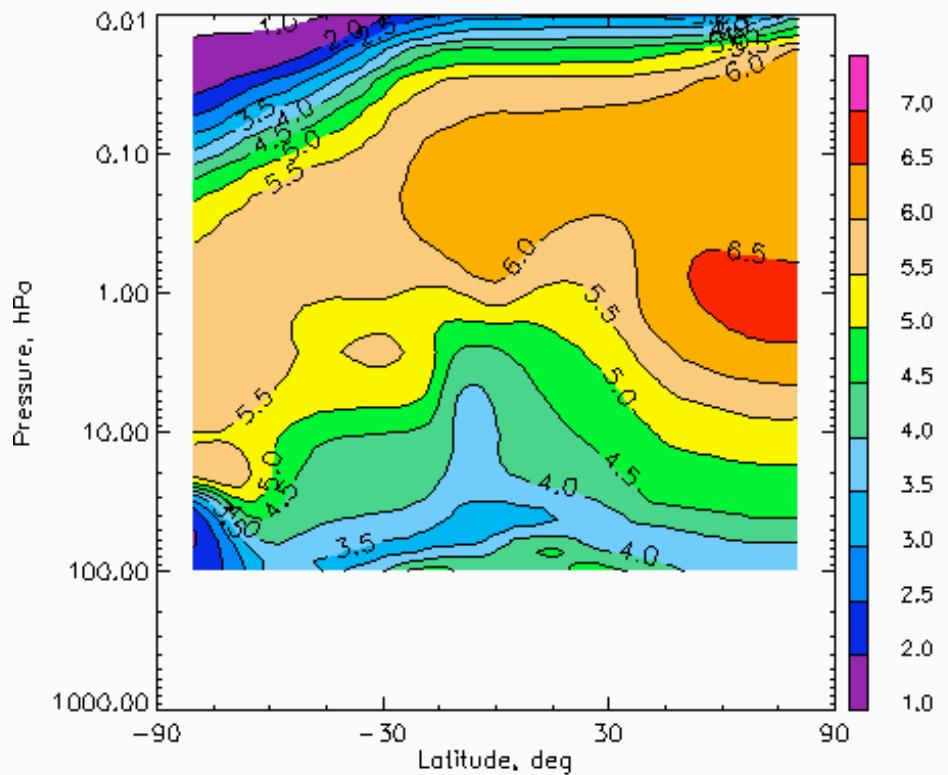
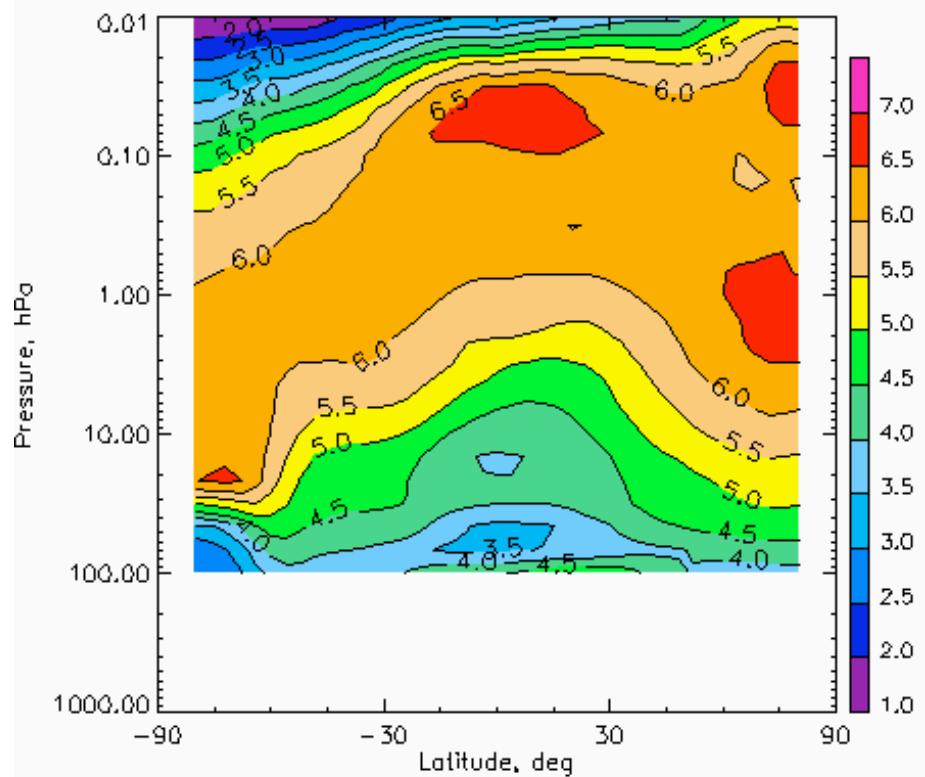
Randel et al., JGR, 2001

# $\text{H}_2\text{O}$ (WACCM2)

Stratosphere / Mesosphere Distribution \*\*\* September

HALOE/MLS

WACCM3

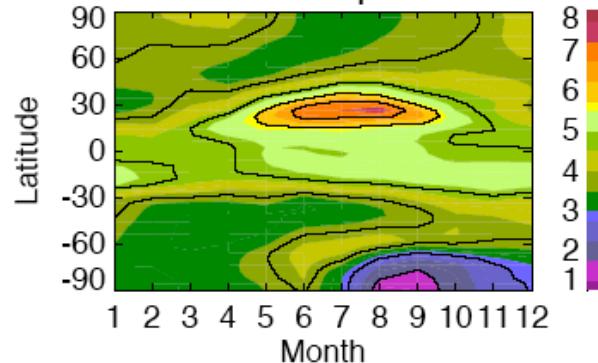


Randel et al., JGR, 2001

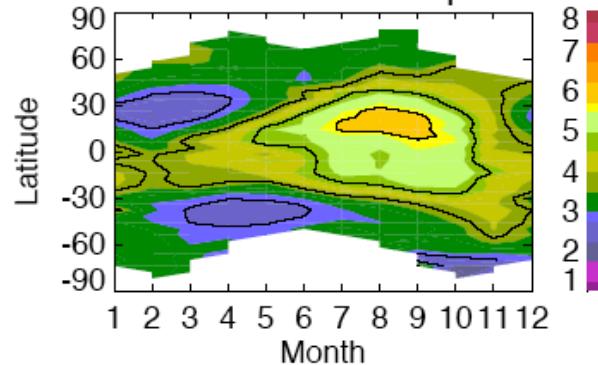
# $\text{H}_2\text{O}$ (ppmv)

## 118 hPa

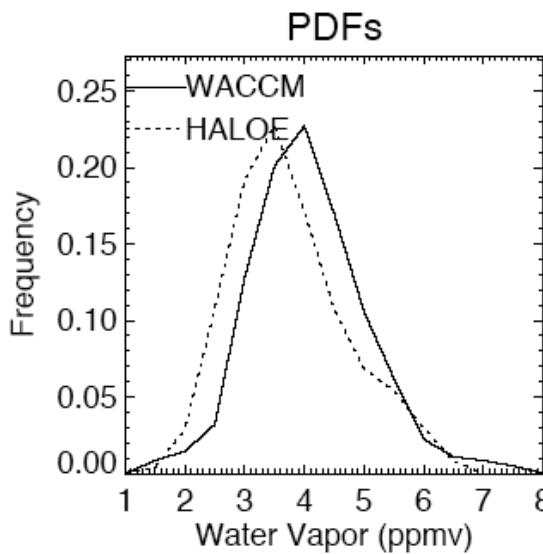
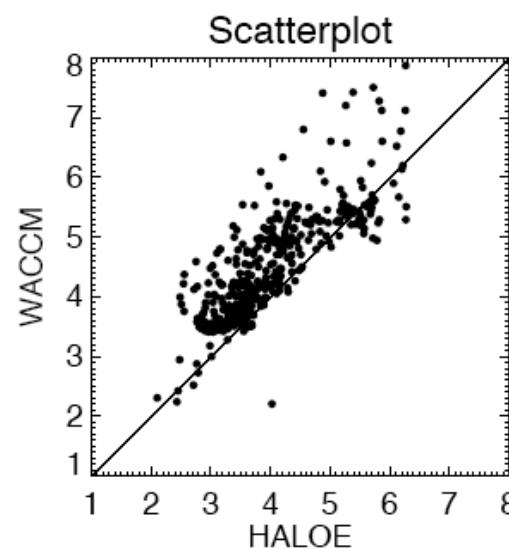
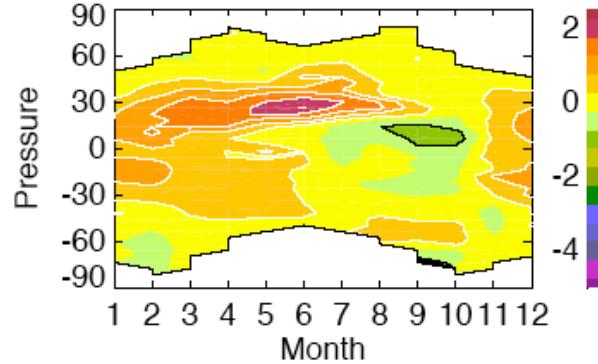
WACCM Water Vapor at 118 hPa



HALOE Water Vapor

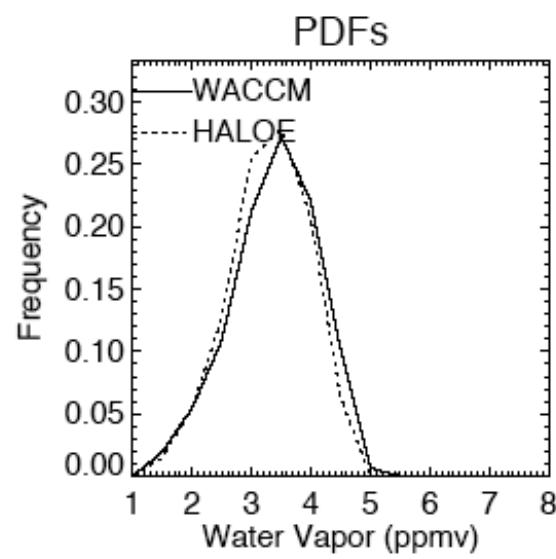
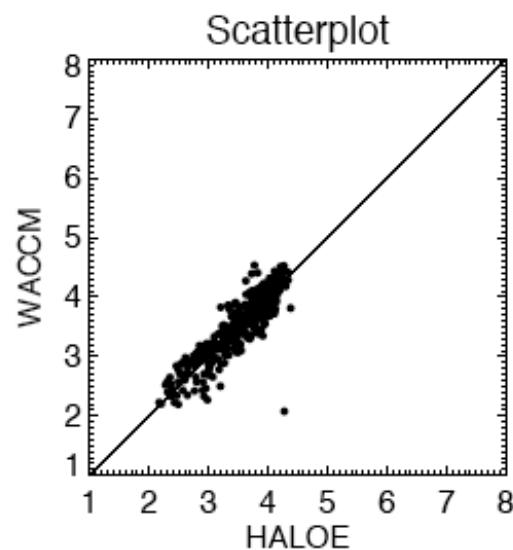
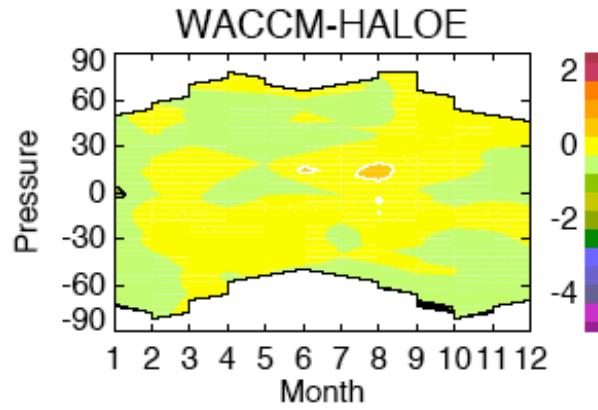
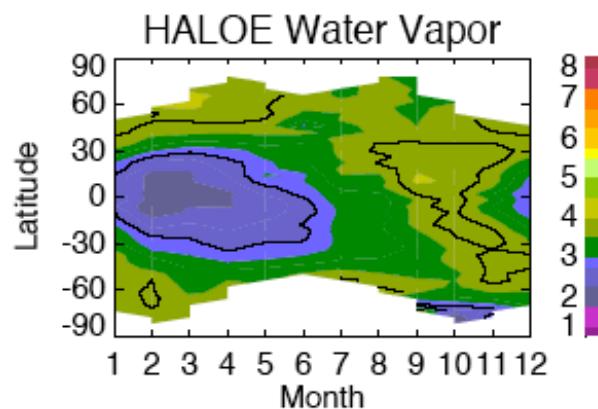
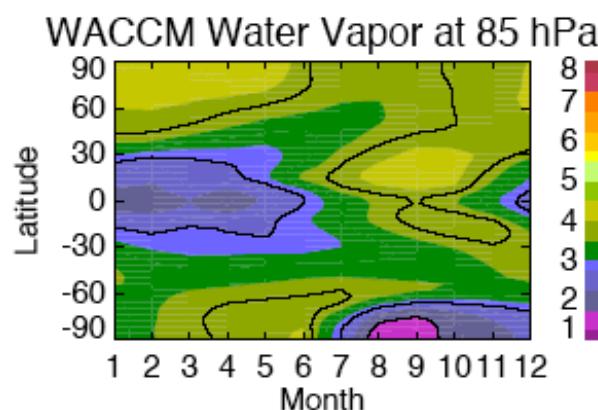


WACCM-HALOE



# $\text{H}_2\text{O}$ (ppmv)

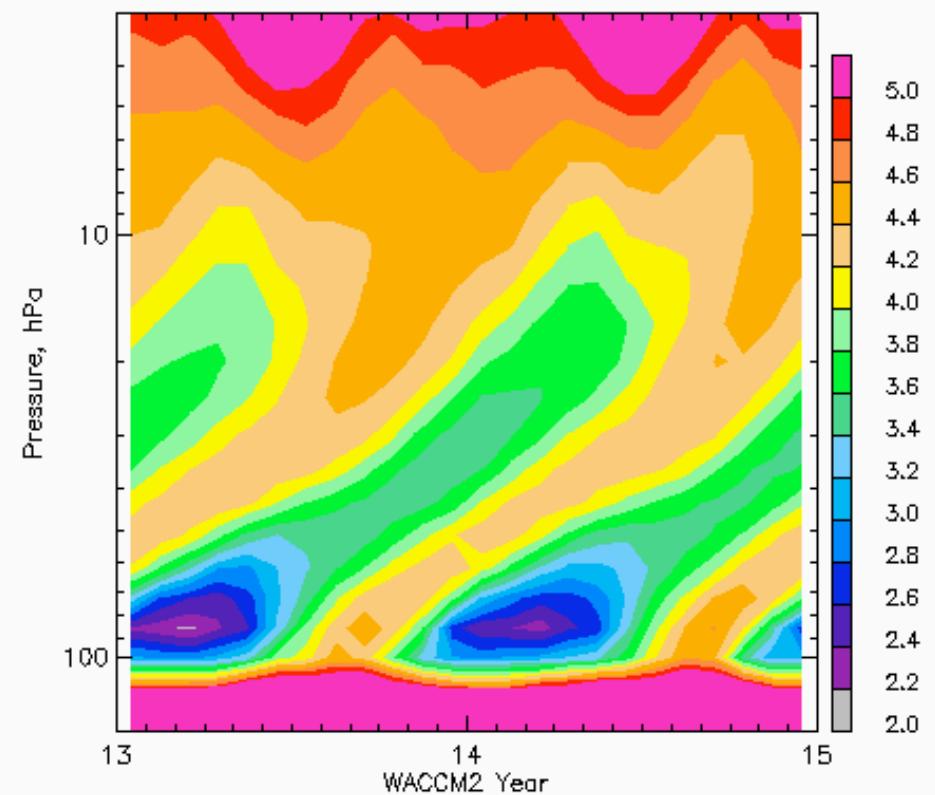
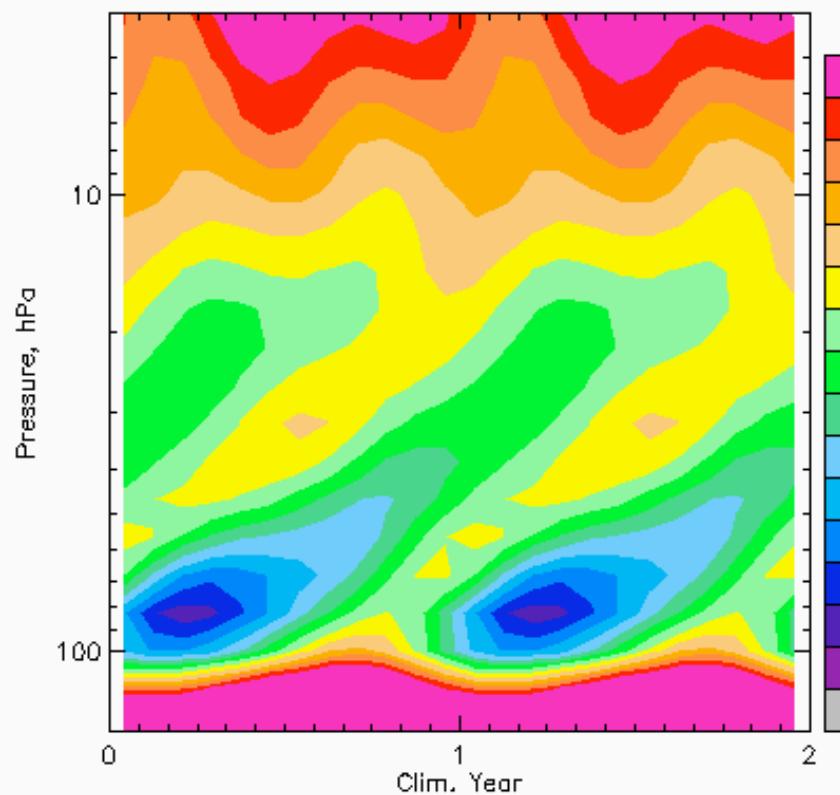
## 85 hPa



# $\text{H}_2\text{O}$ - Tape Recorder, EQ Region

HALOE

WACCM3

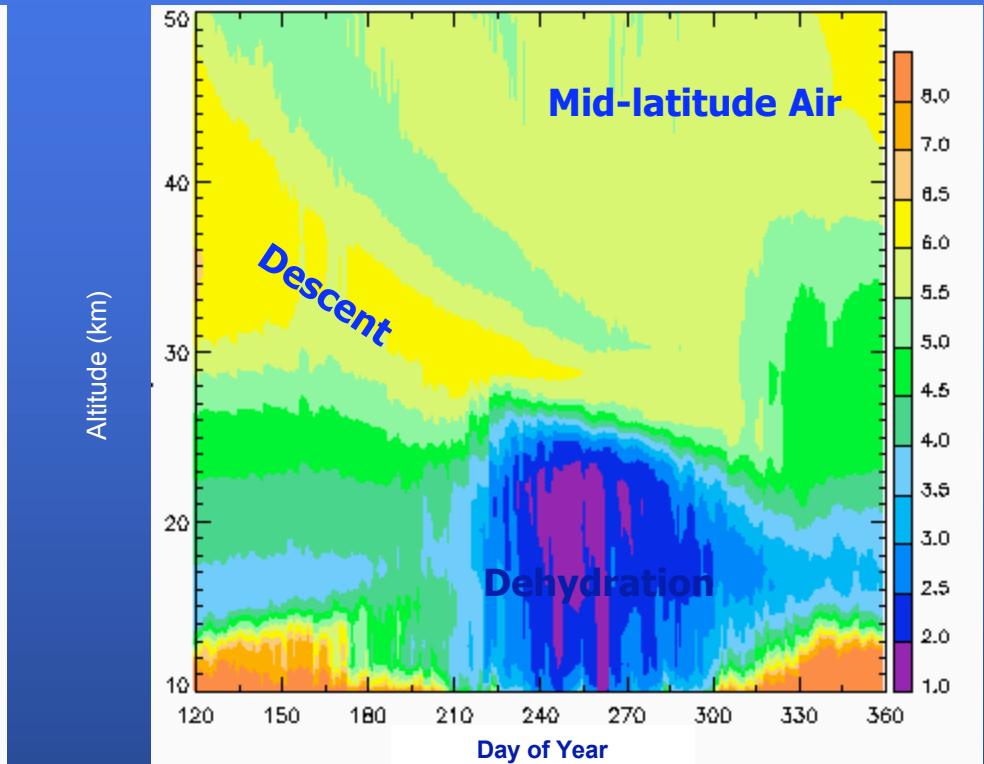
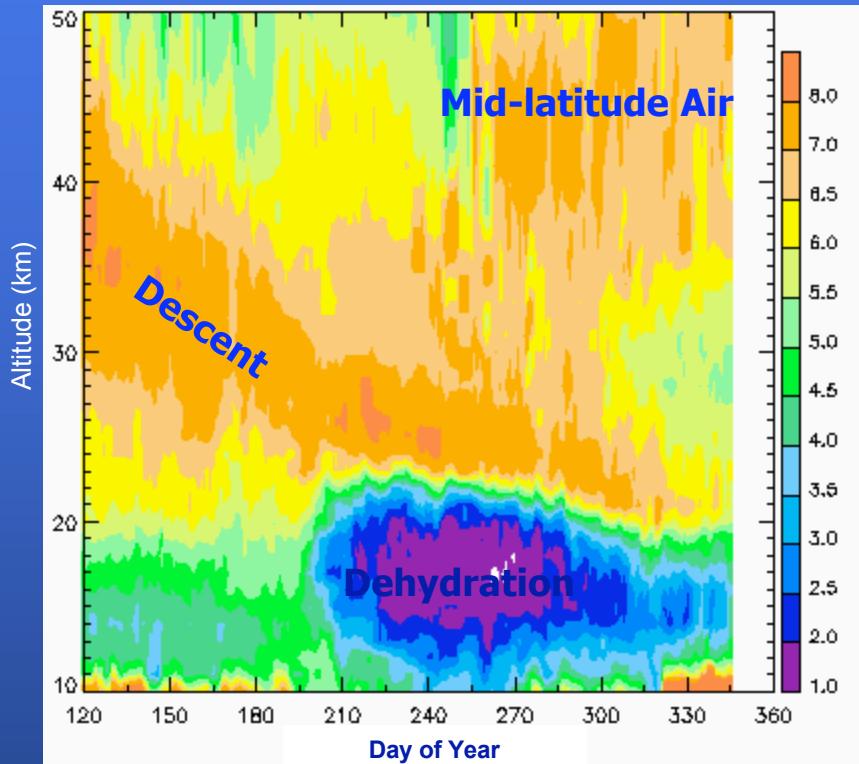


Randel et al., JGR, 2001

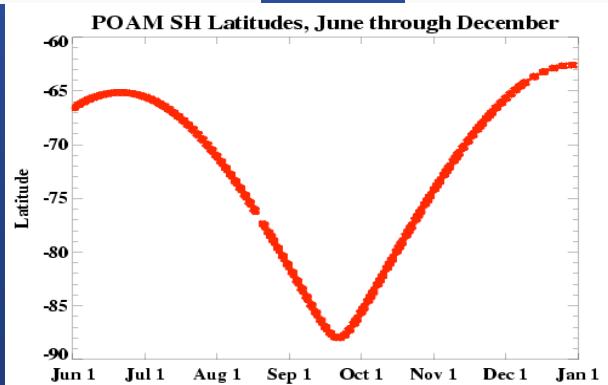
# $H_2O$ SH- Dehydration

POAMIII, 1998

WACCM2 (sampled like POAMIII)



WMO 2002, Figure 3-19,  
Nedoluha et al., 2000.



**Describe Model Components**

**Evaluation with Observations**

**H<sub>2</sub>O trend results**

**Discuss future direction**

# **ENSO Influence on H<sub>2</sub>O Trend**

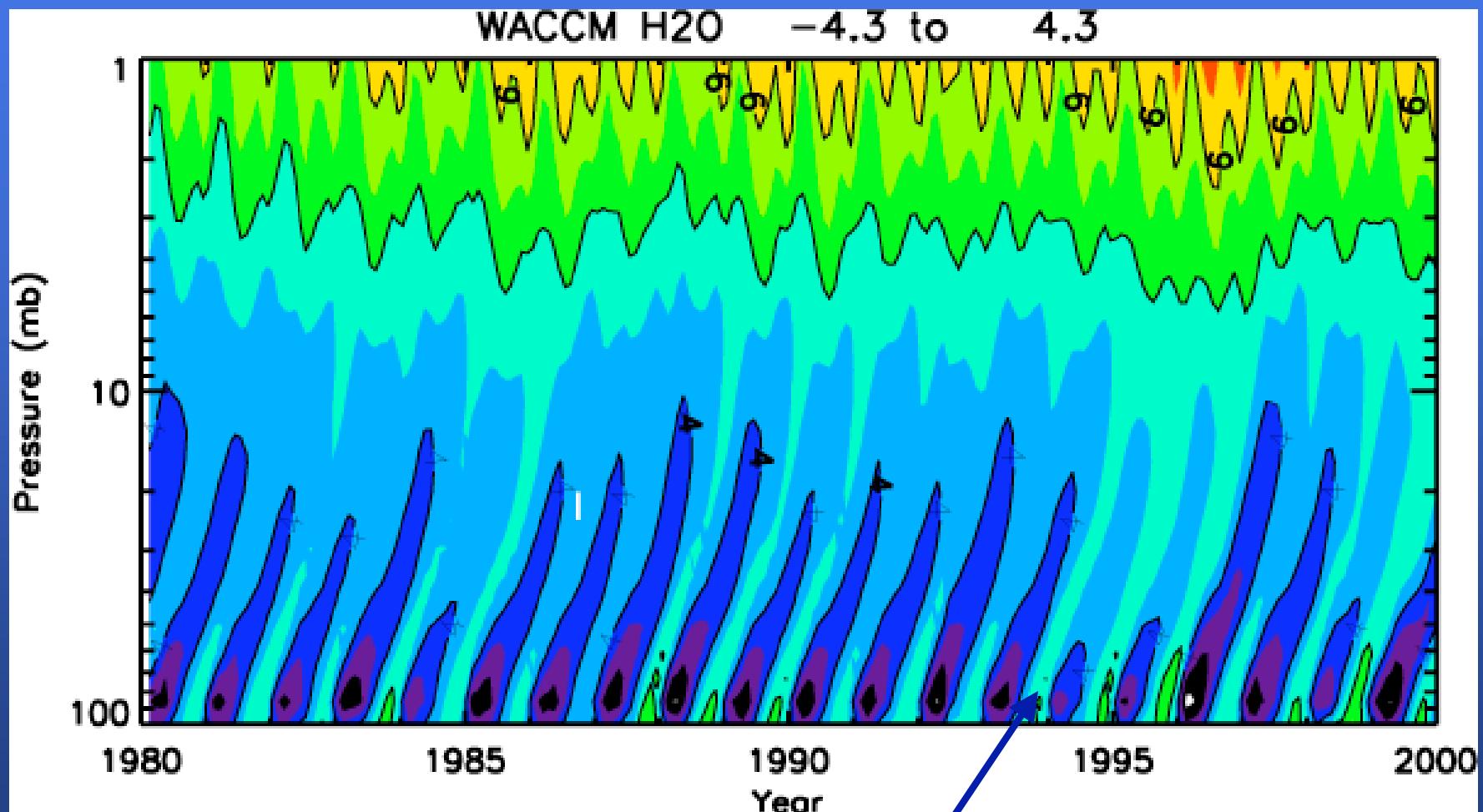
**Marsh, Garcia, Sassi, Kinnison, Boville, et al., 2004.**

## **Model Simulation:**

- WACCM1b was run with time-dependent SST from 1950 through 2000 specified from observations (along with GHG's).
- High frequency output was obtained and used to drive MOZART3 (CCM3.6 column physics from MATCH).
- Time-dependent source gases and stratospheric aerosols were varied in MOZART3 from 1979 to 2000.

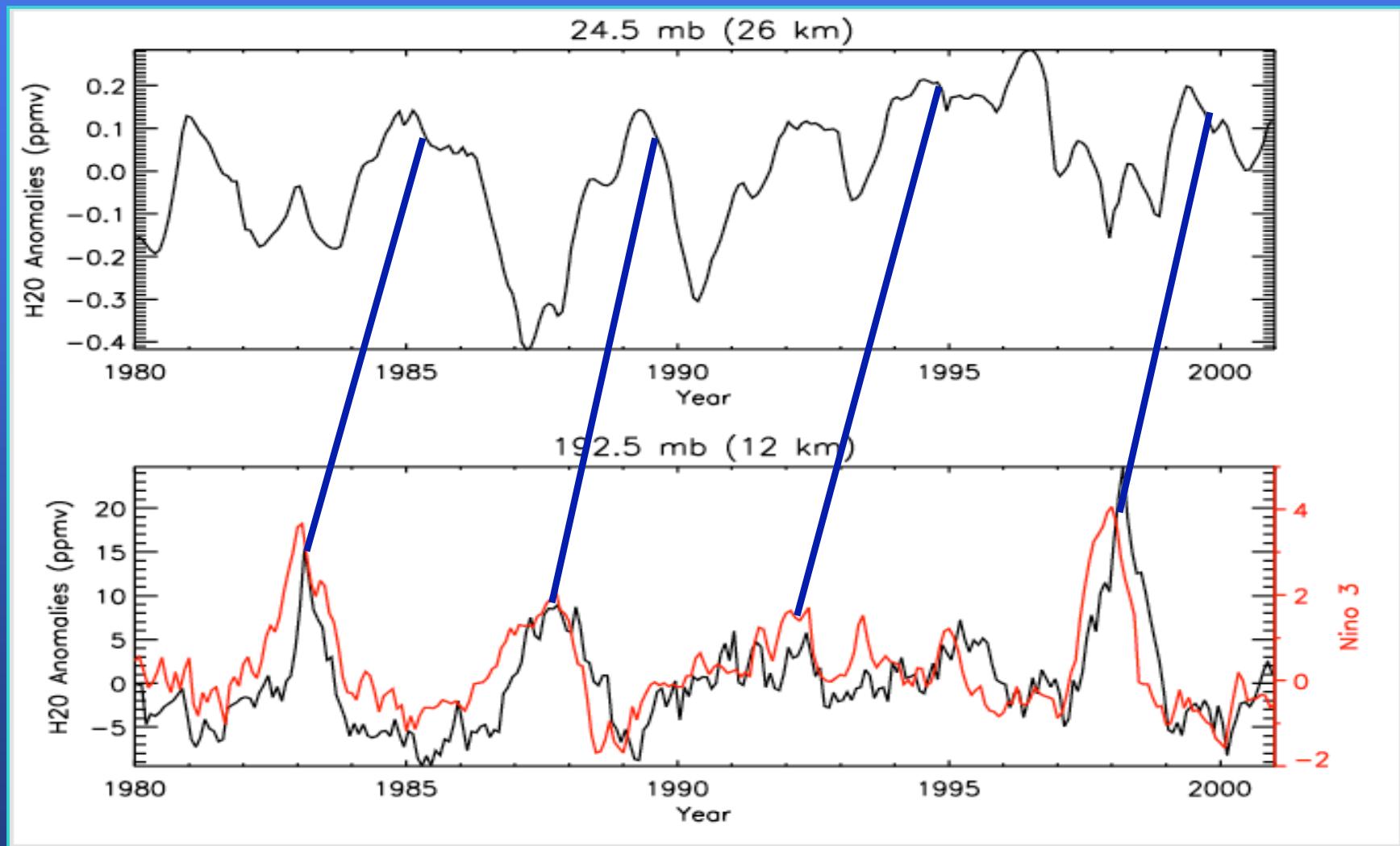
**Short term variability and trends were derived.**

# Representation of H<sub>2</sub>O Trends



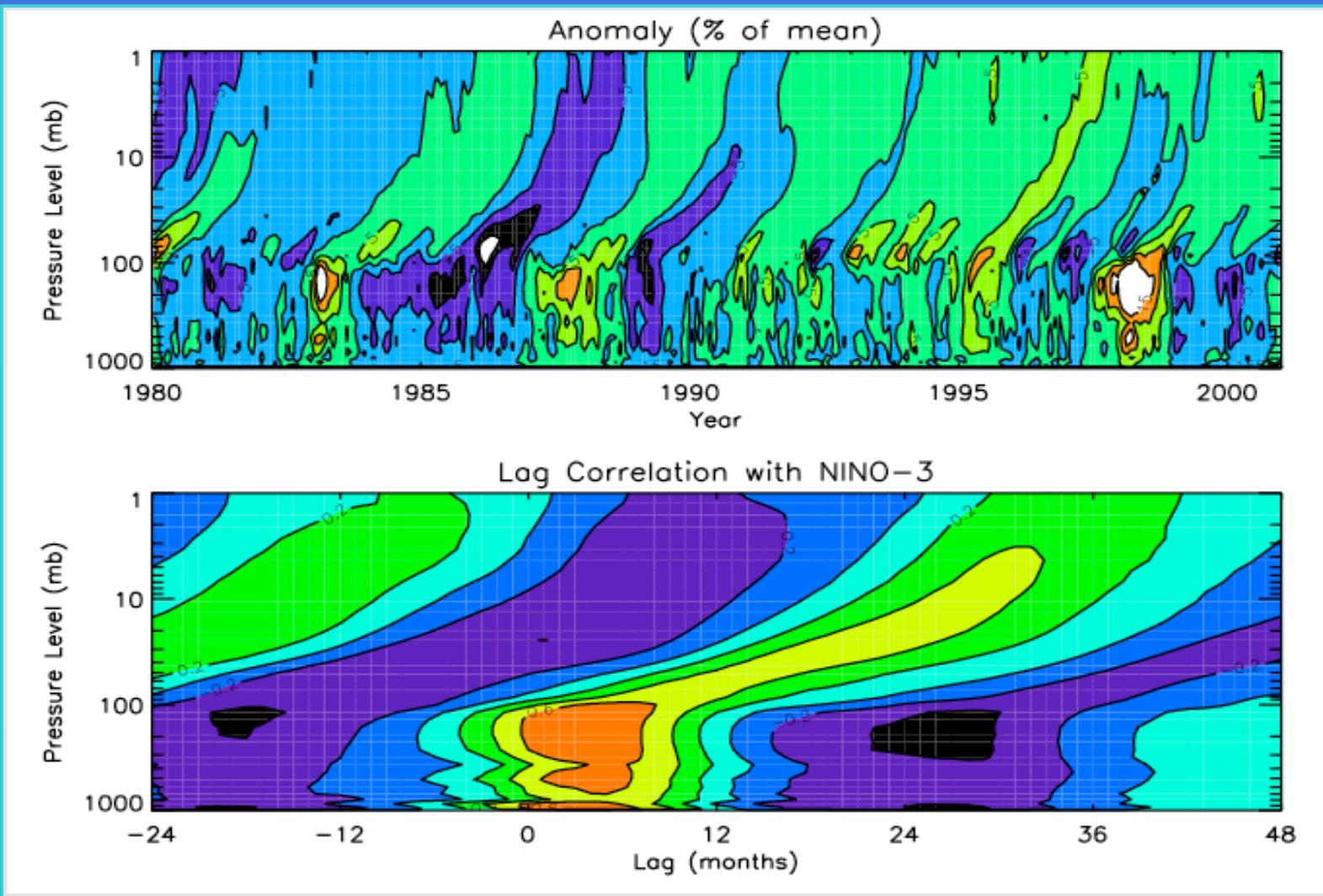
tape recorder + low-frequency variability (+ trend?)

# WACCM1b/MZ3 water vapor

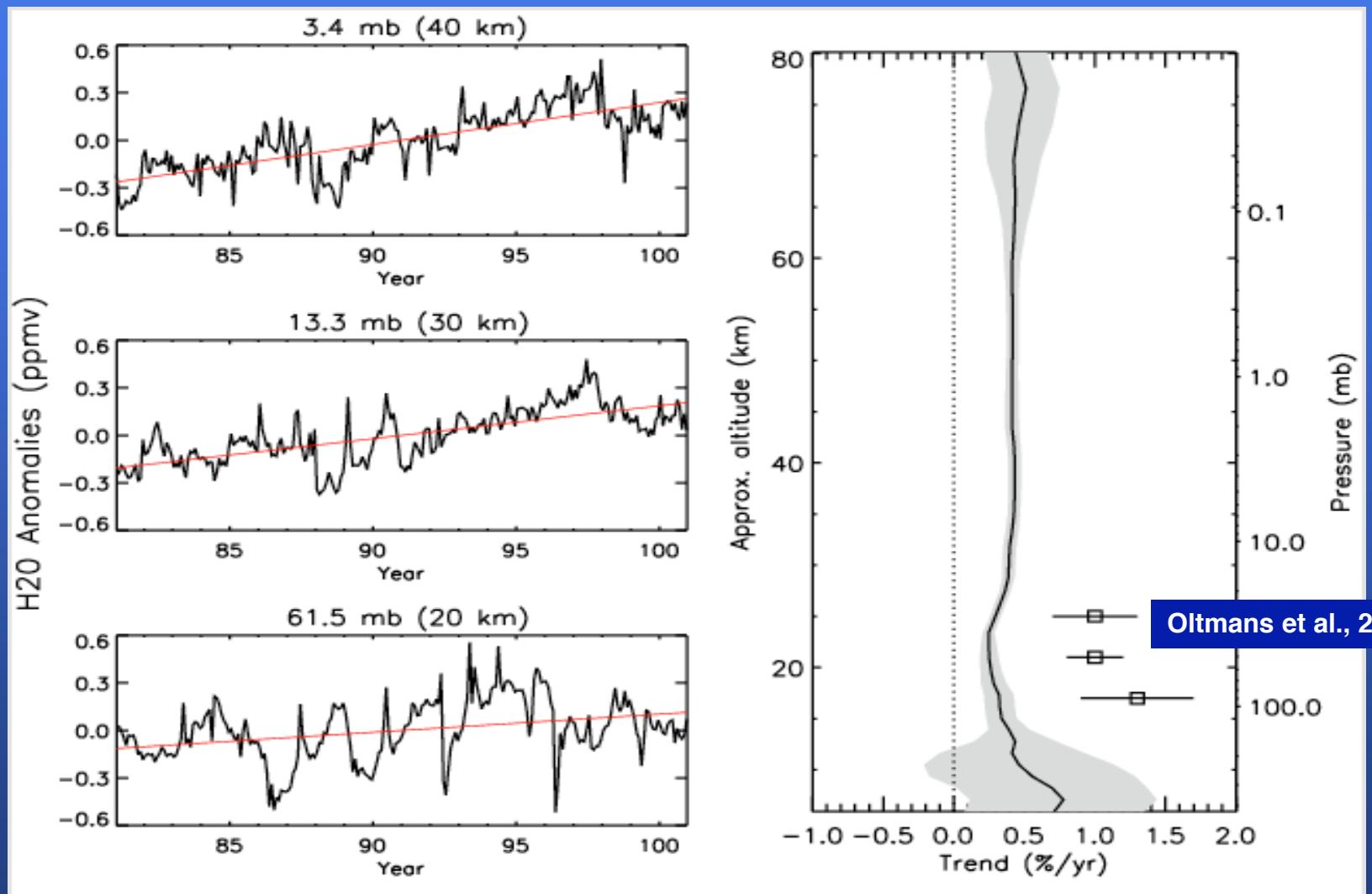


- In WACCM, **low-frequency variability** in lower stratosphere is linked to ENSO

# Correlation with NINO-3 Index



# Modeled trend over Boulder (40N, 105W)



**Describe Model Components**

**Evaluation with Observations**

**Show Ozone and H<sub>2</sub>O trend results**

**Discuss future direction**

# Process Oriented Validation of Chemistry/Climate Models



- Sponsors: DLR / SPARC / GRIPS / PCMDI .
- Leads: Veronika Eyring (DLR), Niel Harris, Markus Rex, Ted Shepperd, D. Fahey, J. Austin, M. Dameris, H. Graf, T. Nagashima, B. Santer, R. Salawitch et al...
- Motivation: “the need to evaluate the skill of coupled chemistry-climate models to predict the future state of the ozone layer.” ... “Need to validate these processes by comparison with observations and other models”.
- SPARC Newsletter, #22, January 2004.
- <http://www.pa.op.dlr.de/workshops/ccm2003/>

**The End**